



NARODOWE CENTRUM NAUKI

UMO-2016/22/E/ST3/00553

Electrical characterization of semiconductors and semiconductor based structures

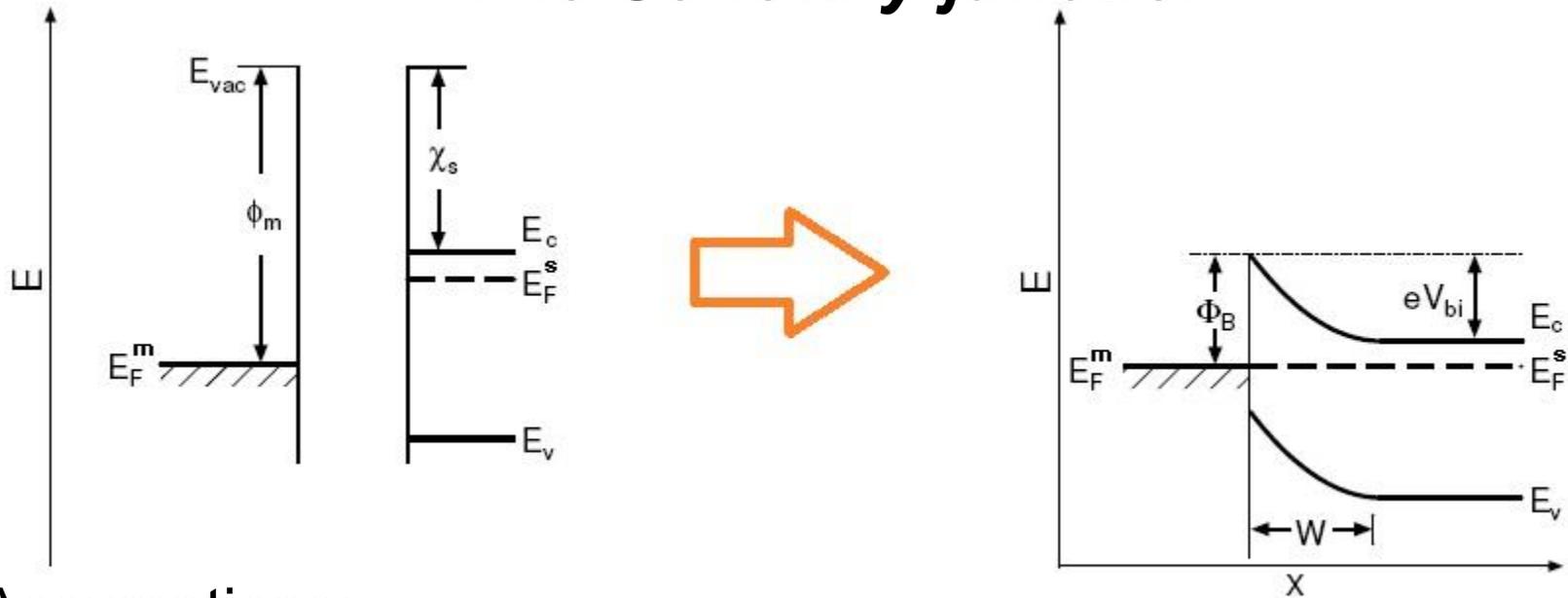
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Outline pt.1

1. Schottky junctions: Schottky-Mott limit and beyond.
2. Rectifying vs. Ohmic contacts and real structures.
3. Current vs Voltage and Capacitance vs Voltage characterization of rectifying structures and what can be extracted from them.

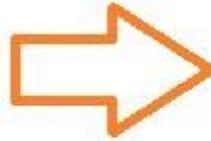
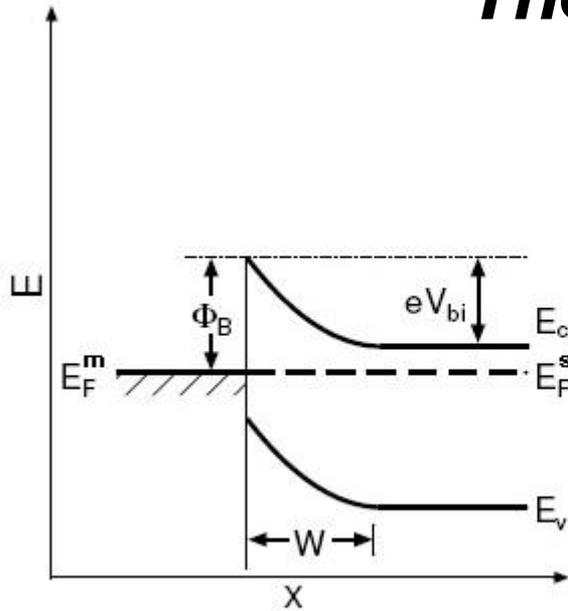
The Schottky junction



Assumptions:

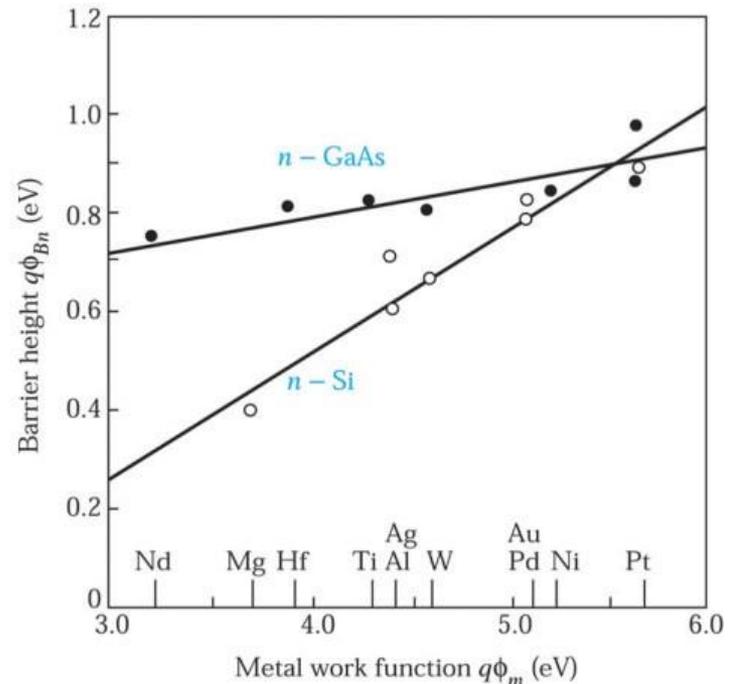
- 1) No changes in ϕ_m and X_s when brought in contact.
- 2) No electron states present on the semiconductor surface or metal-semiconductor interfaces.
- 3) No interfacial layer.

The Schottky-Mott limit



$$\phi_B = \phi_m - \chi_s$$

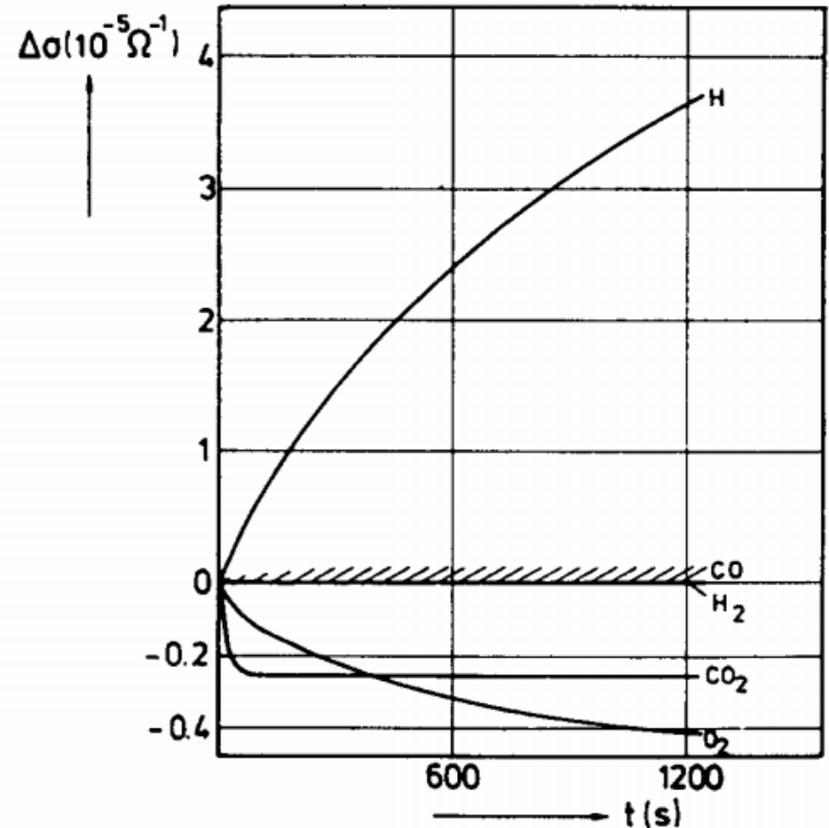
- Case of n-Si the real dependence on ϕ_m is sublinear (~ 0.25).
- Case of n-GaAs ~ 0.1 (0.07).



Surface effects

Examples of effects not considered:

- 1) Adsorbates (difficult to get rid of, like H).
- 2) Sub surface defects resulting from processing, piezo-electric field induced charge/defects.
- 3) Interfacial reactions.
- 4) Formation of surface/interface states and surface reconstruction.



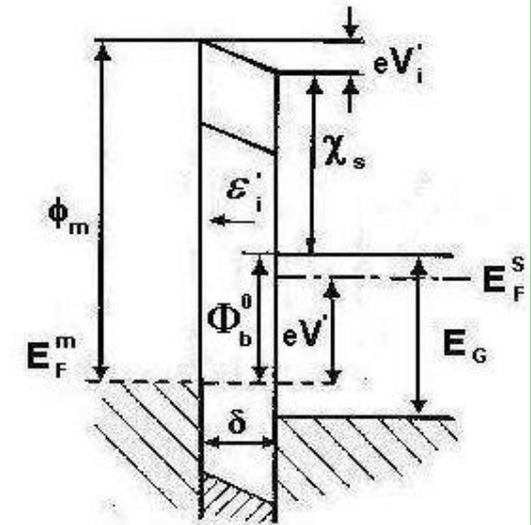
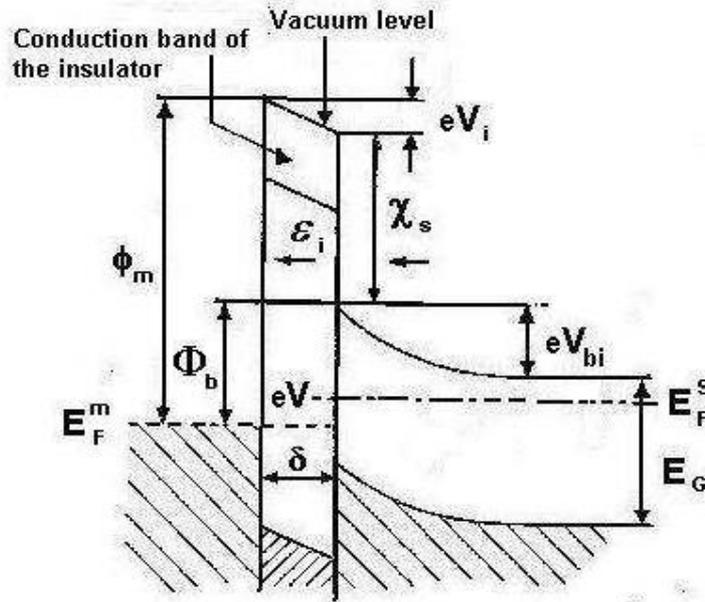
Changes in surface conductivity vs time after exposure of the ZnO (10.0) surface to various gases.*

(*) After V. E. Henrich and P. A. Cox The surface science of metal oxides, Cambridge University Press (1996).

Beyond the Schottky-Mott limit: Bardeen model

Assumptions:

- 1) Interfacial layer of thickness δ .
- 2) Defects in the band-gap uniform D_S (per surface unit and multiplied by e)



$$\Phi_b^0 = \gamma (\phi_m - \chi_s) + (1 - \gamma) (E_G - \phi_0)$$

$$\gamma = \frac{\epsilon_0 \epsilon_r}{\epsilon_0 \epsilon_r + e \delta D_S}$$

with ϕ_0 being the neutral level

$$D_S \rightarrow 0$$

$$\Phi_b^0 = (\phi_m - \chi_s)$$

$$D_S \rightarrow +\infty$$

$$\Phi_b^0 = (E_G - \phi_0)$$

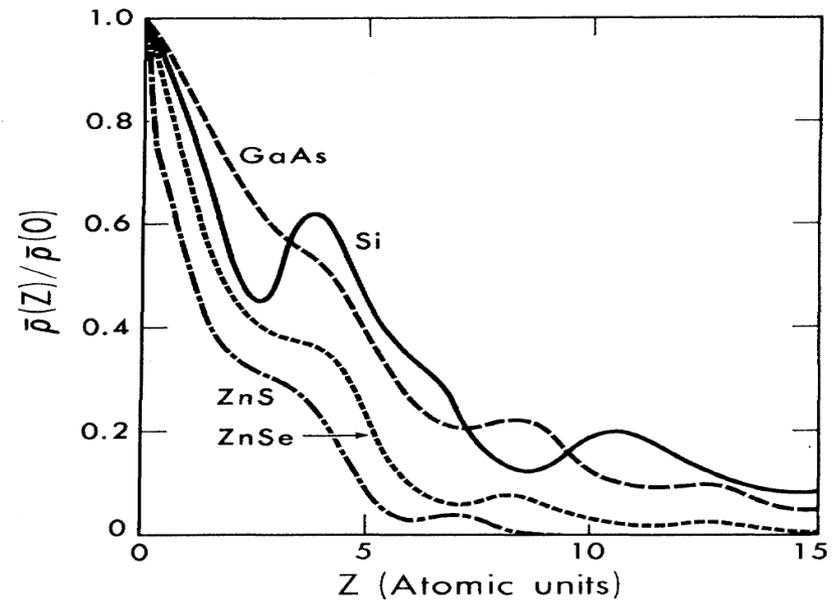
Beyond the Schottky-Mott limit: MIGS model

Assumptions:

- 1) Metal in intimate contact with the semiconductor (i.e. no interfacial layer metal deposited in situ/cleavage).
- 2) Formation of interfacial states by contact with the metal (metal induced gap states-MIGS).



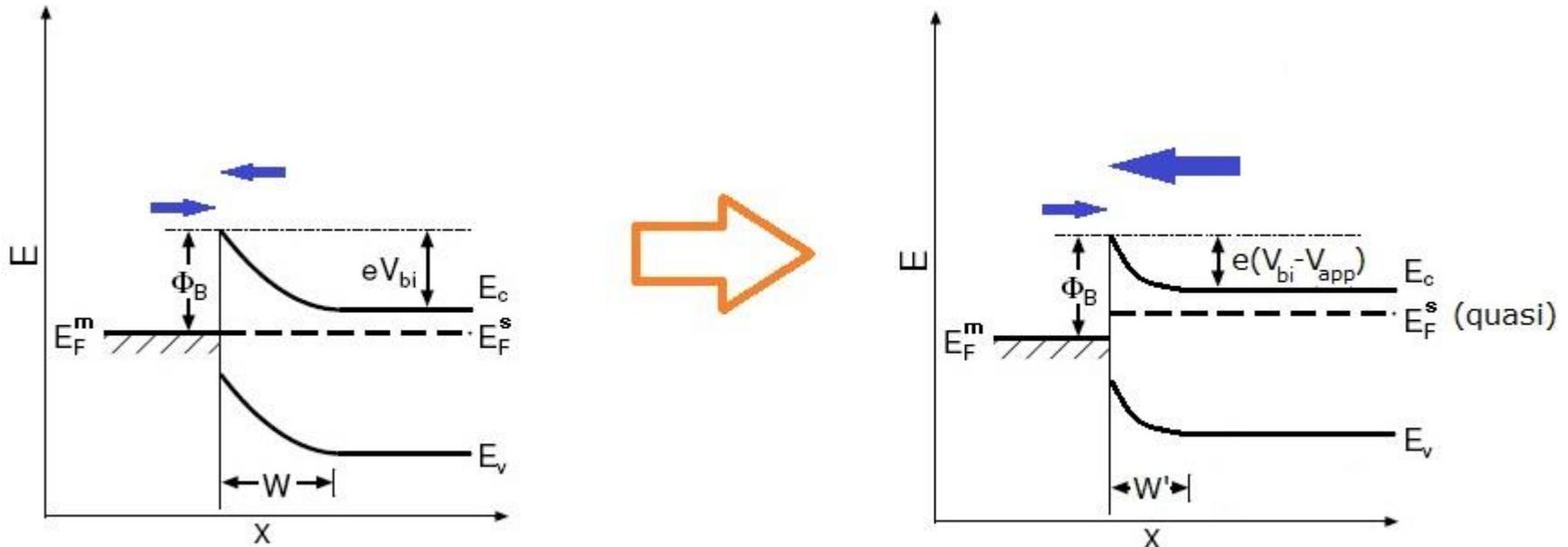
Higher ionicity \rightarrow less penetration \rightarrow towards the Schottky-Mott limit



Relative charge distribution of the MIGS states as a function of the distance from the metal -semiconductor interface ($z=0$). Aluminium used as contact material.*

(*) After S. G. Louie et al. Phys. Rev. B 2154, 15 (1977).

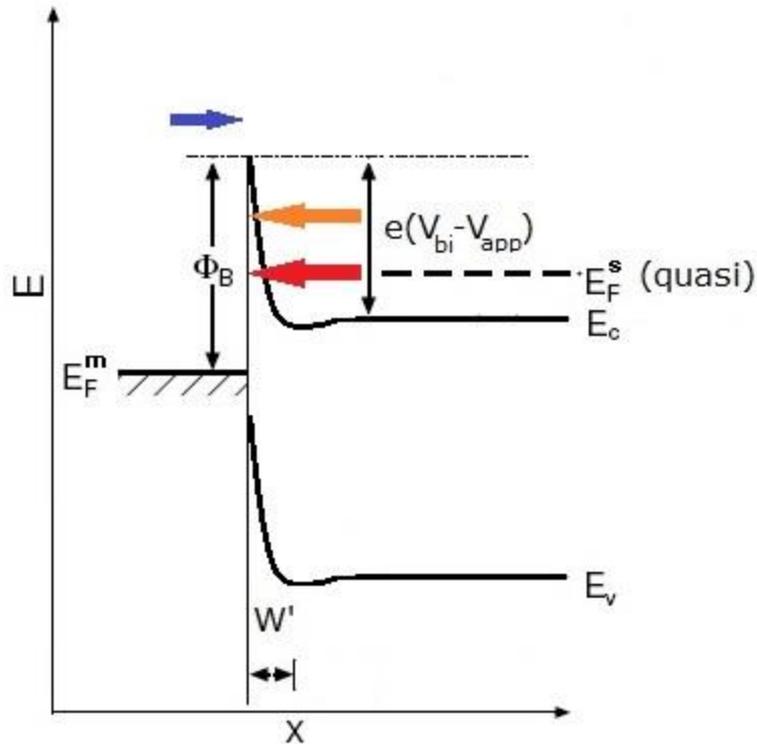
Current in Schottky junctions (thermionic case)



- Flow S→M increase of electrons able to overcome the barrier due to the applied V.
- Flow M→S no changes.

$$J = J_0 \left[\exp\left(\frac{eV}{k_B T}\right) - 1 \right] \quad \text{with:} \quad J_0 = A^* \exp\left(\frac{-e\Phi_{b0}}{k_B T}\right) \quad A^* = \left(\frac{4\pi m^* e k_B^2}{h^3}\right)$$

Rectifying versus Ohmic contacts



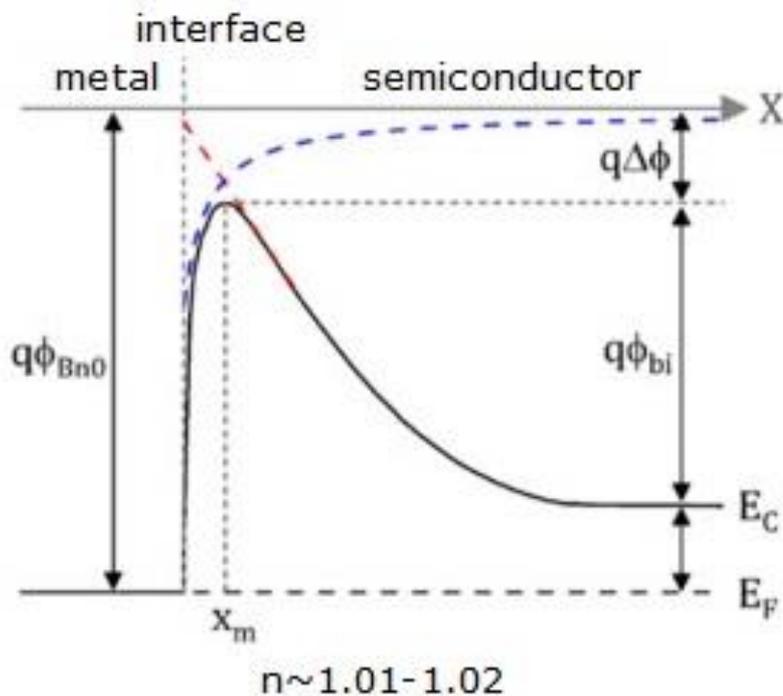
- Reducing the barrier thickness increases the probability of quantum mechanical tunneling.
- For $N_d \gtrsim 10^{17} \text{ cm}^{-3}$
 - 1) Thermionic field emission.
 - 2) Field emission.
- Essentially Ohmic contacts are obtained even though a barrier is present.

Ideality factor n

$$J = J_0 \left[\exp\left(\frac{qV}{k_B T}\right) - 1 \right] \quad \text{with} \quad J_0 = A^* \exp\left(\frac{-e\Phi_{b0}}{k_B T}\right)$$

If the barrier height depends linearly on the applied voltage:

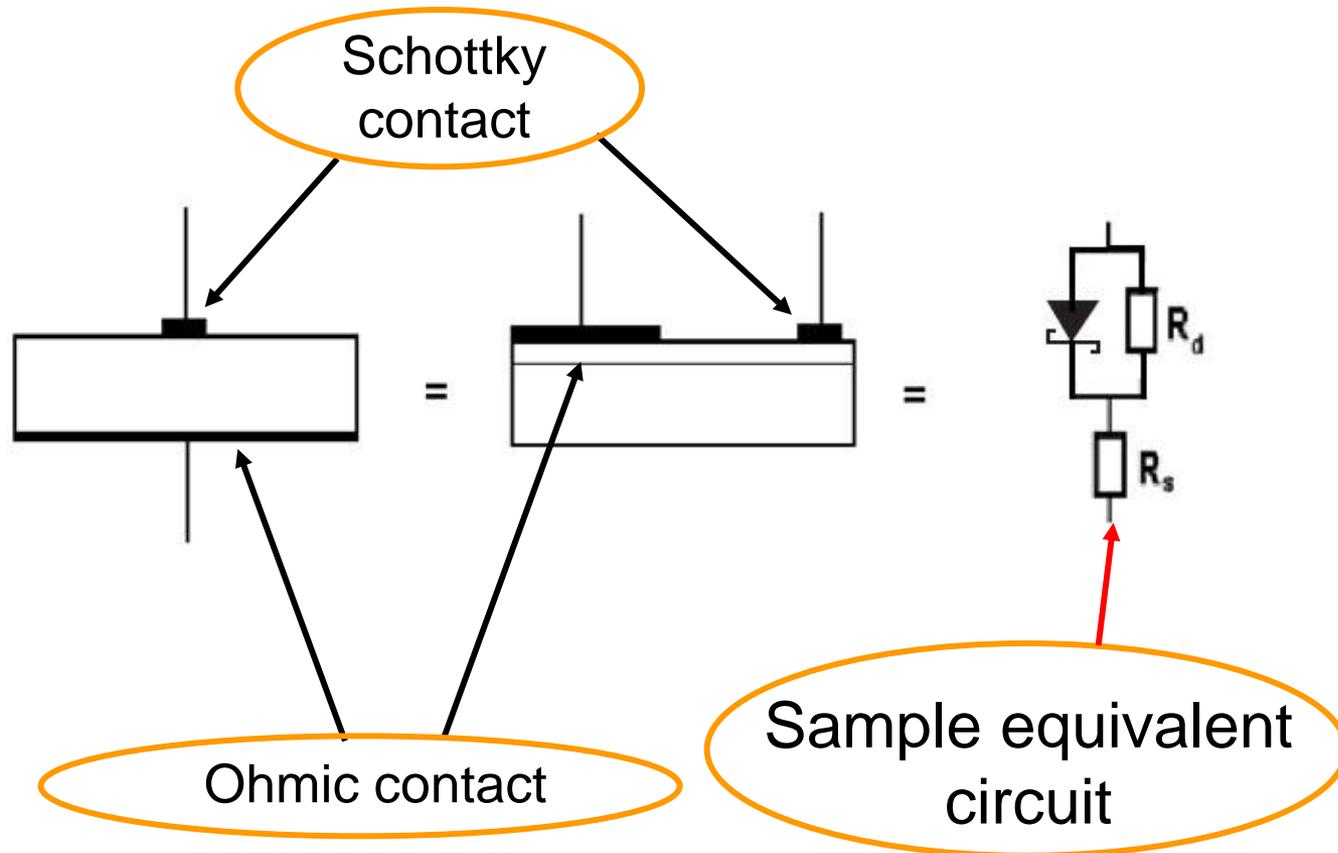
$$J = J_0 \exp\left(\frac{eV}{nk_B T}\right) \left[1 - \exp\left(\frac{-eV}{k_B T}\right) \right]$$



Other examples:

- 1) Interfacial layer.
- 2) Barrier height fluctuations.
- 3) Recombination in the depleted region W ($n \sim 2$).

The real device: equivalent circuit



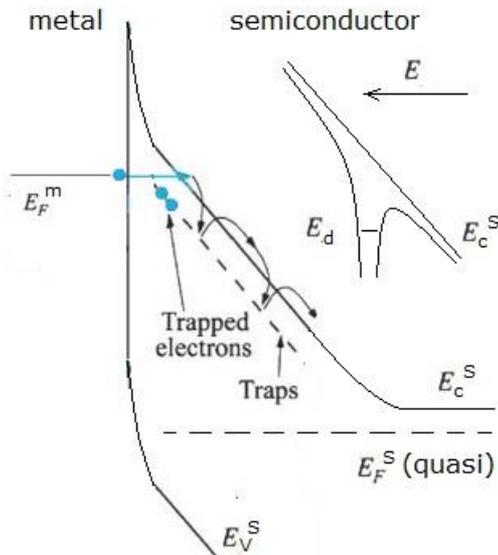
$$I = A J_0 \exp\left(\frac{e(V - IR_S)}{nk_B T}\right) \left[1 - \exp\left(\frac{-q(V - IR_S)}{k_B T}\right)\right] + \frac{(V - IR_S)}{R_d}$$

The leakage mechanism: R_d

- Reverse current characteristics can be analyzed using a differential approach:¹

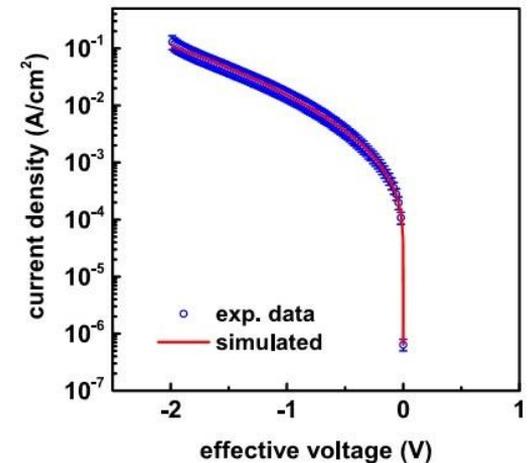
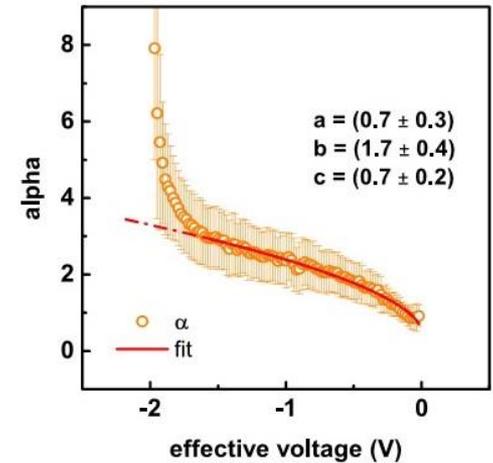
$$\alpha(V) = \frac{V}{I} \frac{dI}{dV} \quad \text{if } I \propto V^a \exp(bV^c) \quad \text{then } \alpha(V) = a + bcV^c$$

- $a \sim 0.5$ points to defective channels conduction and $b \sim 2$ Frenkel-Poole enhancement.²



[1] G.D. Bagratishvili et al. Phys. Status Solidi A 65, 701 (1981).

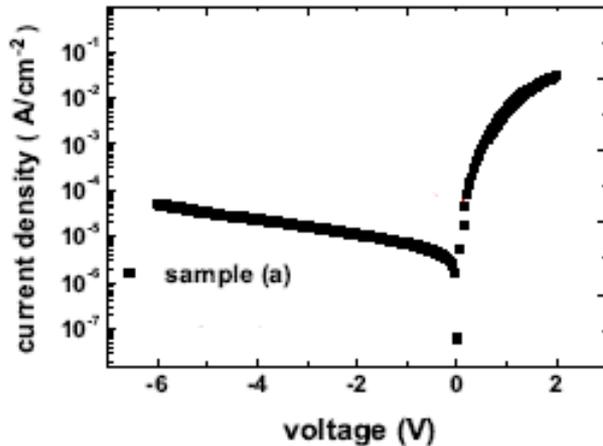
[2] P. Blood, and J.W. Orton, The Electrical Characterization of Semiconductors: Majority Carriers and Electron States, Academic Press, London, 1992.



a	b	c
0.6–0.7	1.2–1.9	0.6–0.7

(*) After R. Schifano et al. Appl. Surf. Science 149067, 552 (2021)).

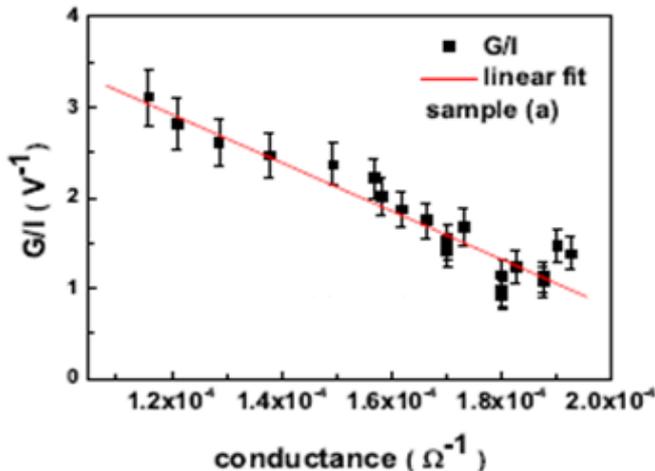
I-V to determine R_S and n (Werner method)



Schottky contact in the thermionic emission regime current with reverse characteristics already analyzed:

$$I = I_0 \exp(e(V - IR_S)/nk_B T)$$

when $e(V - IR_S) \gg k_B T$

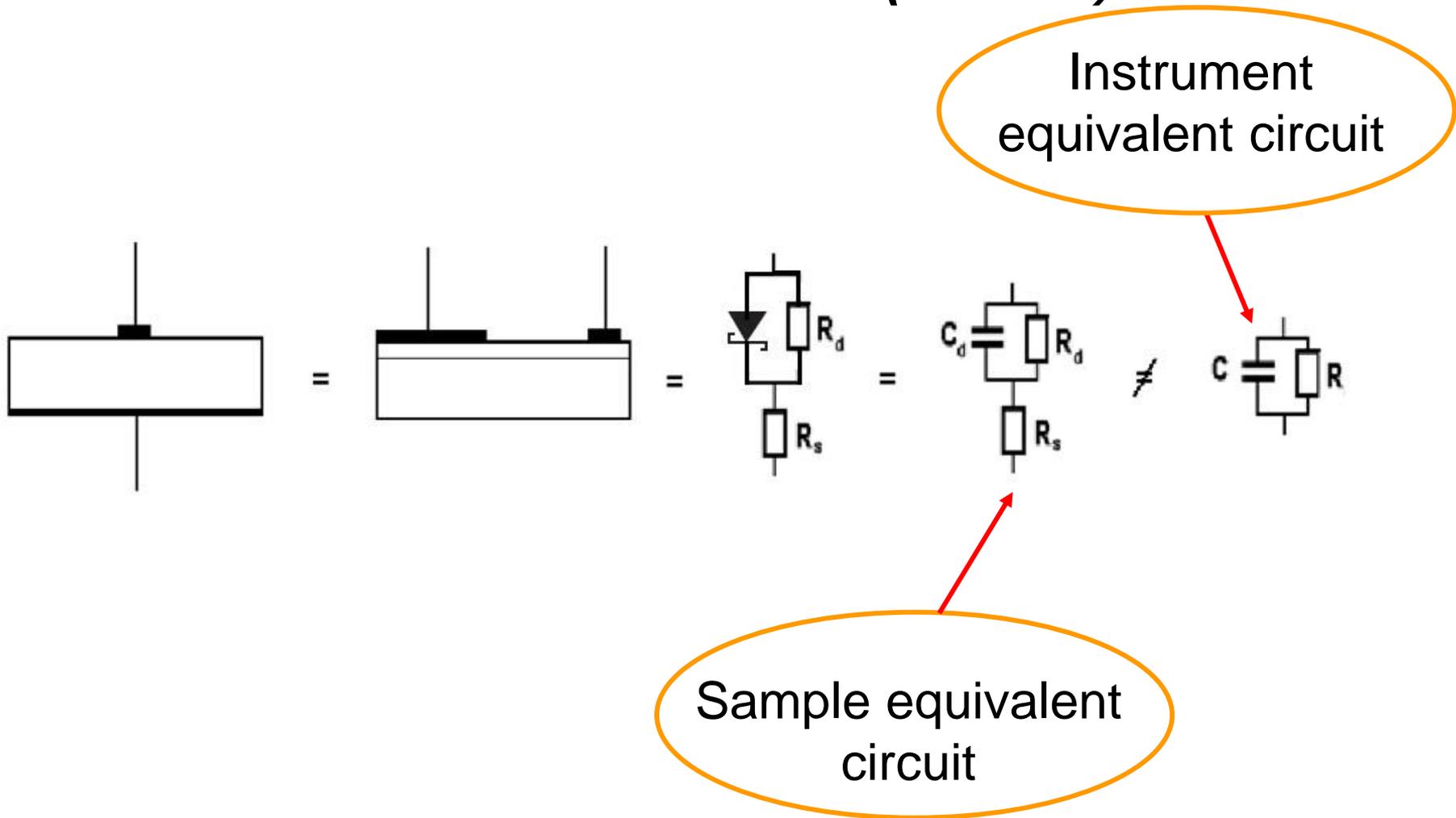


$$\frac{G}{I} = (e/nk_B T)(1 - GR_S)$$

$$n \approx 6$$

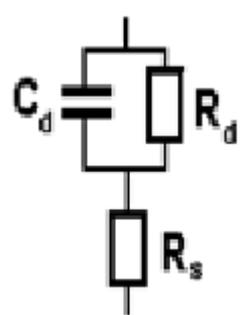
$$R_S = (44 \pm 6) \cdot 10^2$$

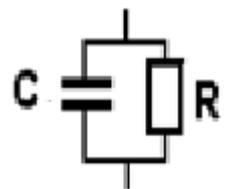
The real device: equivalent circuit reverse bias case (details)



R_S has to be known prior to measure the capacitance.

Effect of R_s on the capacitance measurements


$$C_d \parallel R_d \text{ in series with } R_s = Z^{-1} = \frac{\omega^2 C_d^2 R_s + \frac{1}{R_d} \left(1 + \frac{R_s}{R_d}\right)}{\left(1 + \frac{R_s}{R_d}\right)^2 + \omega^2 C_d^2 R_s^2} + j \frac{\omega C_d}{\left(1 + \frac{R_s}{R_d}\right)^2 + \omega^2 C_d^2 R_s^2}$$


$$C \parallel R = Z^{-1} = \frac{1}{R} + j \omega C$$

$$R_s \ll R_d \quad \omega C_d R_s \ll 1$$



$$C \rightarrow C_d$$

C-V measurement of a Schottky diode

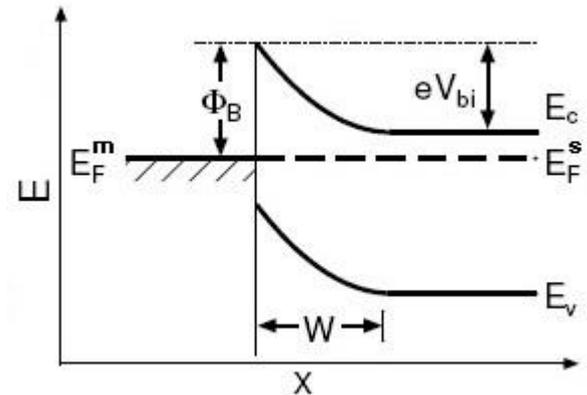
- The capacitance of a Schottky diode vs reverse bias (V_R) in case of constant effective doping ($N_D - N_D$):¹

$$C^{-2} = \left(\frac{2}{A^2 e (N_d - N_a) \epsilon_0 \epsilon_r} \right) \left(V_{bi} + V_r - \frac{k_B T}{e} \right)$$

- Plotting C^{-2} vs V_R can be used to evaluate V_{bi} .



Possibility to measure ϕ_B if $(E_C - E_F)$ can be determined.



C-V measurements to measure the conduction band misalignment

- Anderson model equivalent to the Schottky-Mott limit
- The conduction band offset ΔE_C is given by

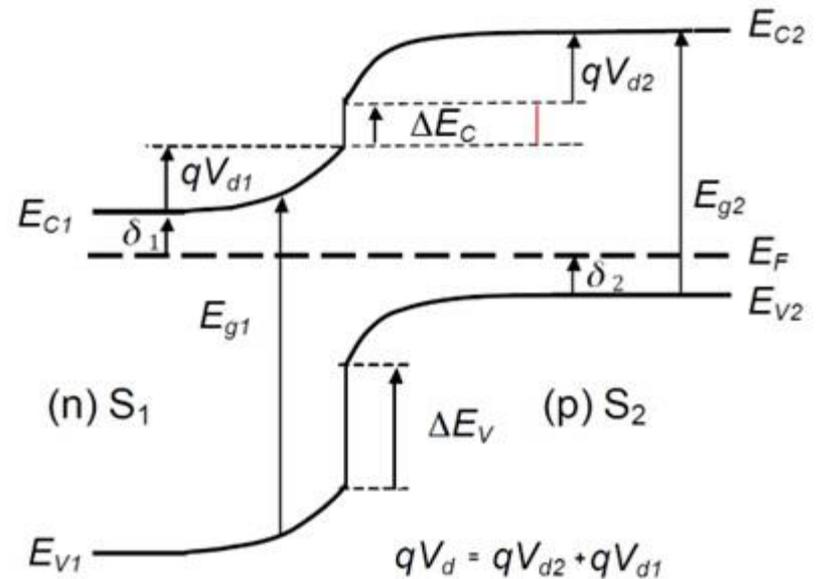
$$\Delta E_C = E_{g2} - (qV_d + \delta_1 + \delta_2)$$

with δ_1/δ_2 equal to

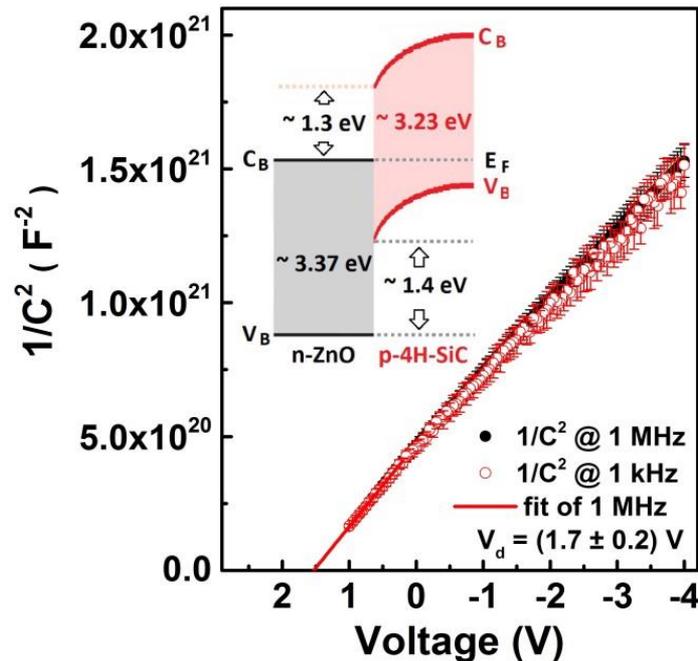
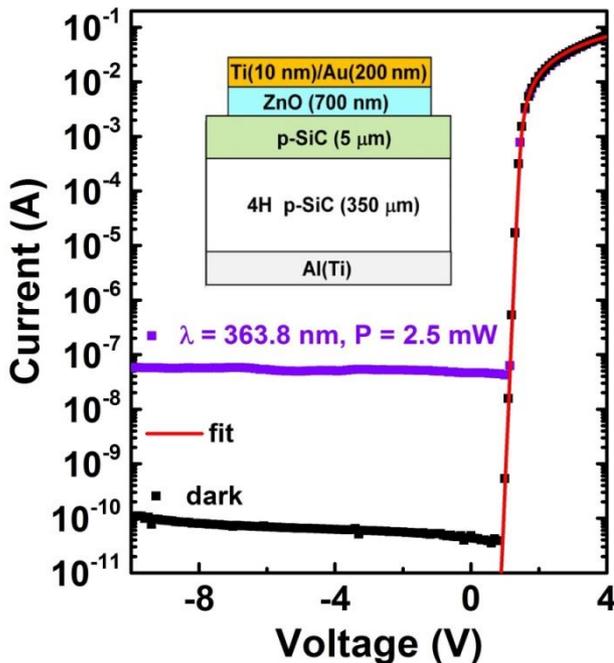
$$n_{S1} = \int_0^{+\infty} \sqrt{2E} \frac{m_{S1}^{3/2}}{\pi^2} \frac{1}{\exp((E + \delta_{S1})/k_B T) + 1} \quad p_{S2} = \frac{1}{4} \left(\frac{2k_B T m_{S2}}{\hbar^2 \pi} \right)^{3/2} e^{-\frac{\delta_{S2}}{k_B T}}$$

and qV_d that can be measured by C-V considering that:

$$C_d = A \sqrt{\frac{e \epsilon_{S1} \epsilon_{S2} n_{S1} p_{S2}}{2(\epsilon_{S1} n_{S1} + \epsilon_{S2} p_{S2})}} \frac{1}{\sqrt{V - V_d}} \quad \Rightarrow \quad \frac{1}{C_d^2} \propto (V - V_d)$$



Example: the n-ZnO/p-4H-SiC heterostructure



(*) After M. Guziewicz, R. Schifano et al. Appl. Phys. Lett. **107**, 101105 (2015).

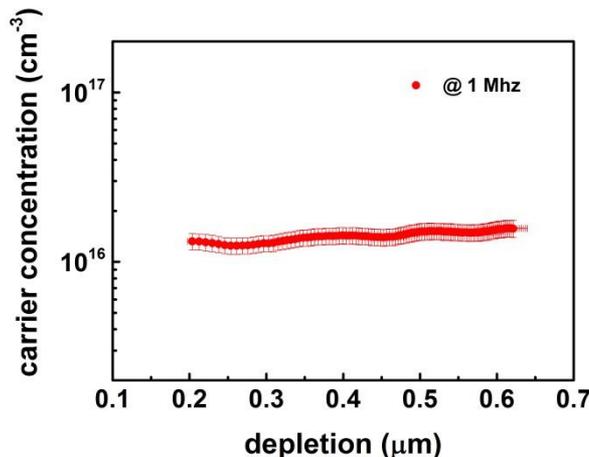
[1] H. B. Fan et al. Appl. Phys. Lett. **92**, 192107 (2008)

- Mesa structures with a semitransparent Al/Ti Ohmic back contact ($\sim 10\%$ transmittance).
- High rectification ratios (10^9), ideality factor ~ 1 (1.17 ± 0.04), leakage current density ($\sim 6 \cdot 10^{-8} \text{ A/cm}^2$), ($\sim 10^3$) light to dark reverse current ratio.
- Type II band alignment, $\Delta E_c = (1.3 \pm 0.2) \text{ eV}$ in agreement with the values extracted from XPS measurements (1.5 ± 0.2) eV.¹

C-V measurement of a Schottky diode: effective donor profile (beyond the uniform approximation)

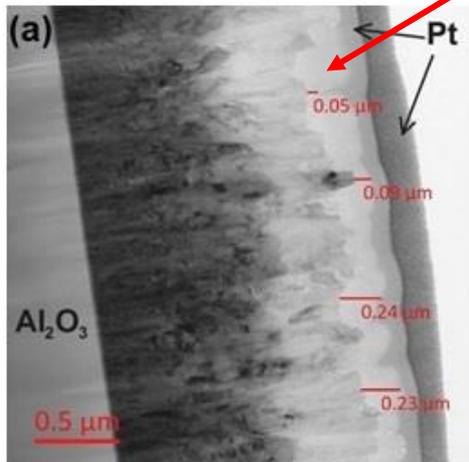
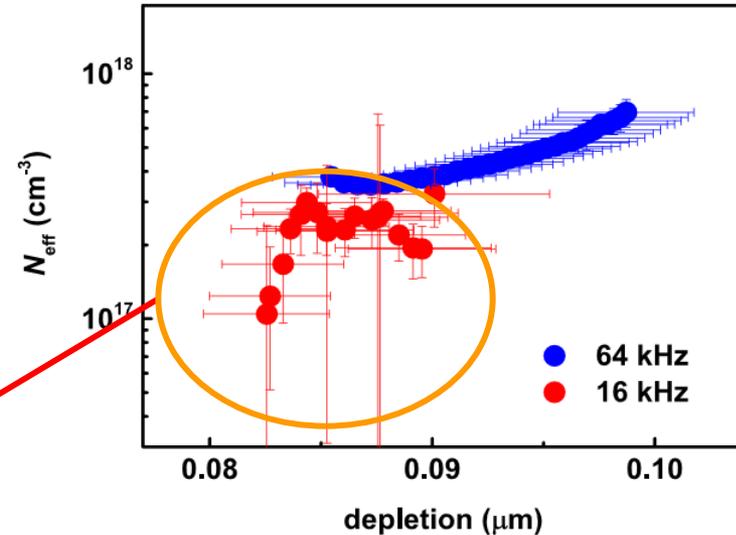
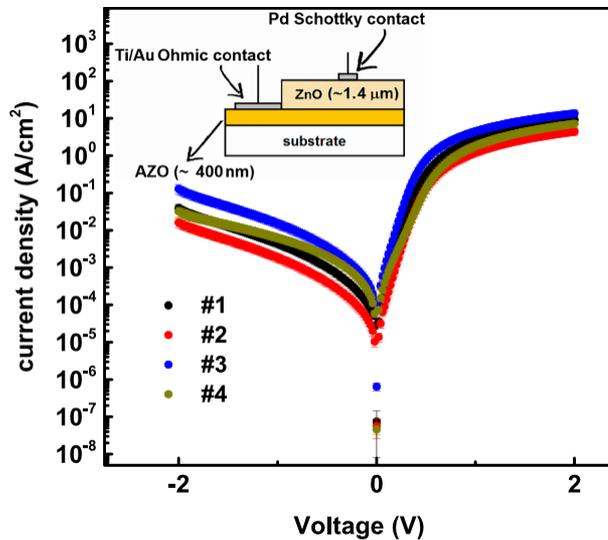
- The profile of the effective donor concentration N_{eff} (electron responding to the probing signal).

$$N_{eff}(W) = \frac{1}{e \epsilon_0 \epsilon_r A^2} \frac{C^3}{\frac{\partial C}{\partial V}} \quad \text{with} \quad W = \frac{\epsilon_0 \epsilon_r A}{C}$$



- The profile of the effective donor concentration N_{eff} in the n-ZnO/p-4H-SiC heterostructure discussed in the previous slide.

Effective donor profile: example



- TEM analysis evidenced presence of an O-rich polycrystalline/amorphous region on the ZnO surface/interface.

- $O_i(\text{oct})/V_{\text{Zn}}$ theoretically anticipated to be acceptor like defects consistent with the N_{eff} profile.¹

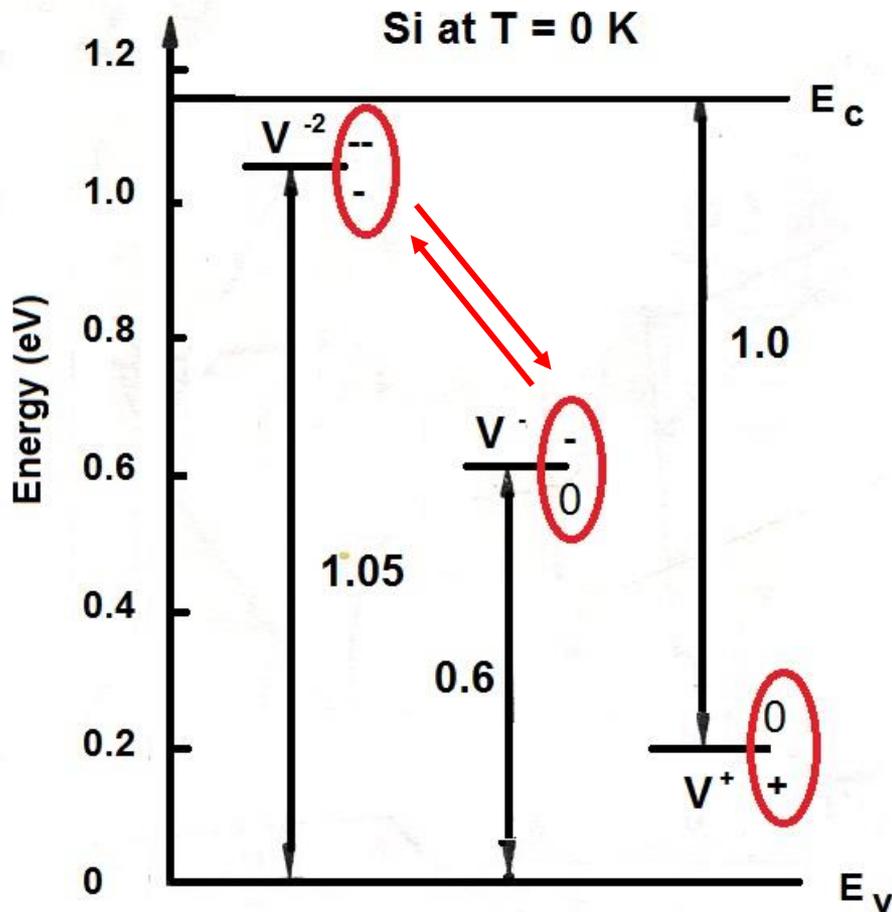
(*) After R. Schifano et al. Appl. Surf. Science 149067, 552 (2021)).

[1] A. Janotti et al., Phys. Rev. B 76, 165202 (2007)

Outline pt.2

1. Defects characteristics.
2. Deep level transient spectroscopy and Laplace deep level transient spectroscopy: how it is working and examples.
3. Thermal admittance spectroscopy: how it is working and examples.
4. Towards electrical defects assignment: examples.

Electrically active defects in a semiconductor (beyond shallow donors)



- Deep levels strongly localized.
- The same defect can present several charge states (provide different levels).
- Adding an electron does not necessary means reducing the enthalpy-activation energy (negative-U).

Interaction of a defects with the bands

- Capture of carriers occurs via a characteristics quantity, the capture cross section, via

$$c_n = \sigma_D \langle v \rangle n$$

- Emission towards the bands follows an exponential emission law

$$e_n^D = \sigma_{Di} T^2 \gamma \exp\left(\frac{-E_D}{k_B T}\right) \quad \text{with} \quad \gamma = 2\sqrt{3} (2\pi)^{\frac{3}{2}} k^2 \frac{m m^*}{h^3}$$

$$e_n^D / c_n \simeq \exp\left(\frac{E_D - E_F}{k_B T}\right)$$

Defects: carrier emission/capture

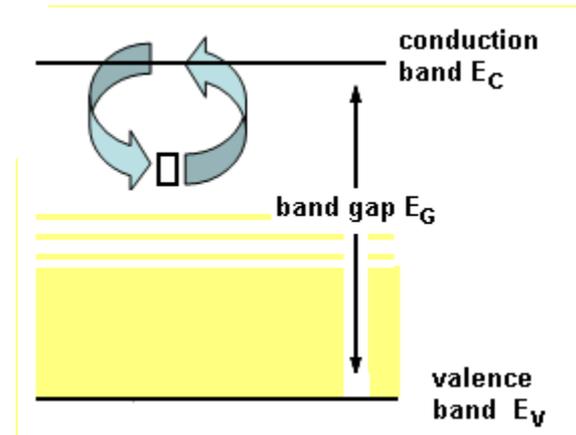
Shockley-Read-Hall statistics for majority carrier trap:

- the defect is emitting mainly towards the closest band.
- capture determined by the Fermi level position respect to the position of the defect related level into the bandgap

n-type semiconductor



majority carriers trap are defects with levels in the upper part of the band gap



TAS/DLTS what can they be used for?

- Determining signatures (capture cross section/enthalpy-activation energy) of electrically active defects and their concentration.
- Based on capacitance measurements.

Requirements for TAS/DLTS

- Relatively good rectifying junction.
- Depletion region extending mainly in the material to be studied i.e. Schottky contacts, n^+ -p or p^+ -n junctions/heterostructures .

Principle of TAS/DLTS measurements

- Study of the changes in capacitance due to the emission/capture of majority carriers by electrically active defects present in the depleted region.
- Capacitance changes acquired at different temperatures either temperature scans or different fixed temperatures depending on the accuracy required.

DLTS: how to get a transient (Schottky diode case)

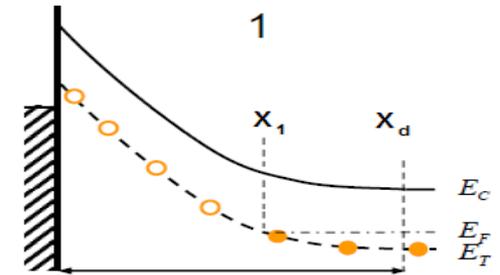
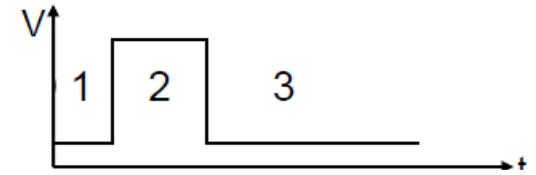
- 1) Steady state: Schottky junction in reverse bias.
- 2) Filling pulse: charging of the defect.
- 3) Back to the initial reverse bias: observing the defect decharging.

$$n_{filled} = N_T \exp(-e_D t) \propto \Delta C(t)$$

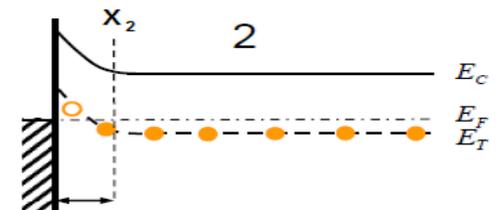
$$e_D = \beta T^2 \sigma_{app} \exp\left(\frac{-\Delta H}{k_B T}\right)$$

$$\Delta C(t) = \underbrace{C_\infty \frac{1}{2} \left(\frac{x_1^2 - x_2^2}{x_d^2} \right)}_{\Delta C_0} \frac{N_T}{N_D} \exp(-e_D t)$$

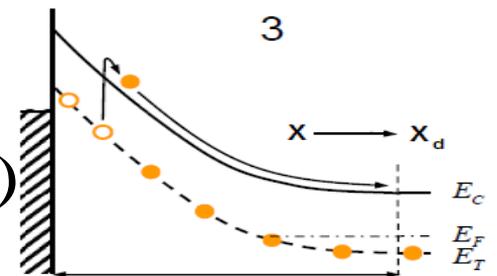
$$N_T \ll N_D$$



Reverse biased junction-steady

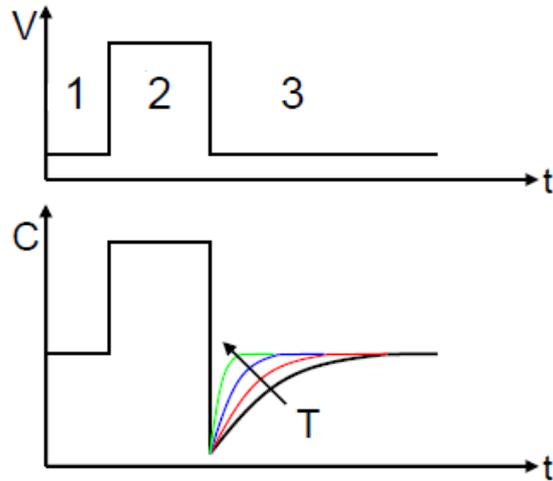


Filling pulse: filling of the defect



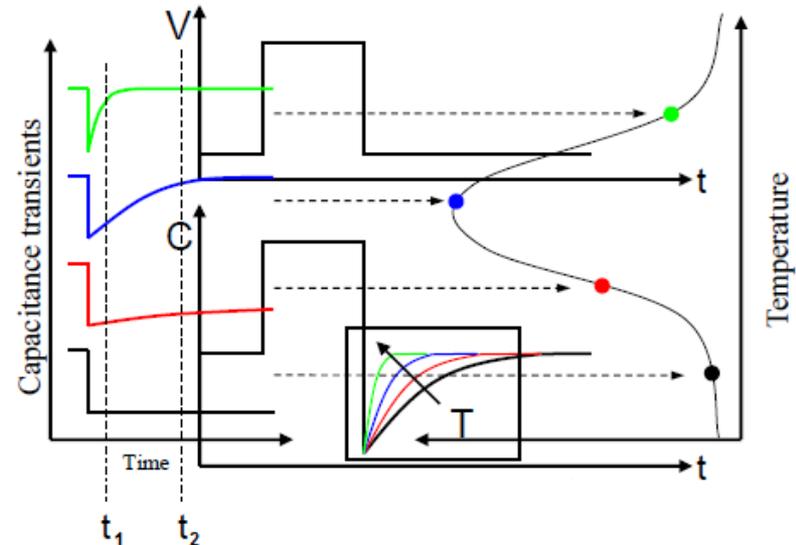
Emission from the defect: transient

DLTS principle how to analyze the acquired data



- Measuring the transients at different temperature.
- The DLTS spectra is the result of post measurement calculations.

- Transient is sampled at time t_1 and t_2 and subtracted*.
- If t_1 fixed and t_2 varied the maximum will shift.



(*) After D. V. Lang J. Appl. Phys. **45**, 3023 (1974)

The DLTS spectra

$$\begin{aligned} S_{DLTS}(T) &= \frac{1}{t_i} \int_{t_p}^{t_p+t_i} \Delta C(t, T) \cdot w(t - t_p) \cdot dt = \\ &= \frac{1}{t_i} \int_{t_p}^{t_p+t_i} \Delta C_0 \exp(-e(T)t) \cdot w(t - t_p) \cdot dt \end{aligned}$$

the weighting function w is establishing the $e(T)$ “window” for which $e(T)$ is “resonant” with the weighting function  DLTS max.

Varying t_i “window” changes the value of $e(T)$ “resonant”.



An Arrhenius plot for $e(T)$ can be constructed

Possible weighting functions (among the others)

- 1) Box-car method (original Lang approach see two slides above).
- 2) Lock-in based on

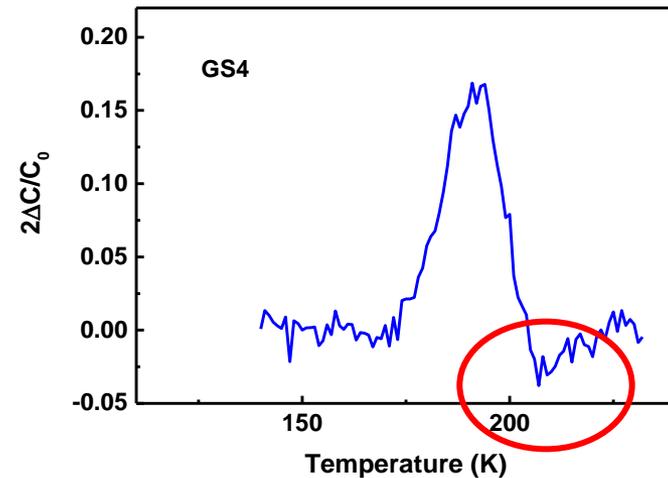
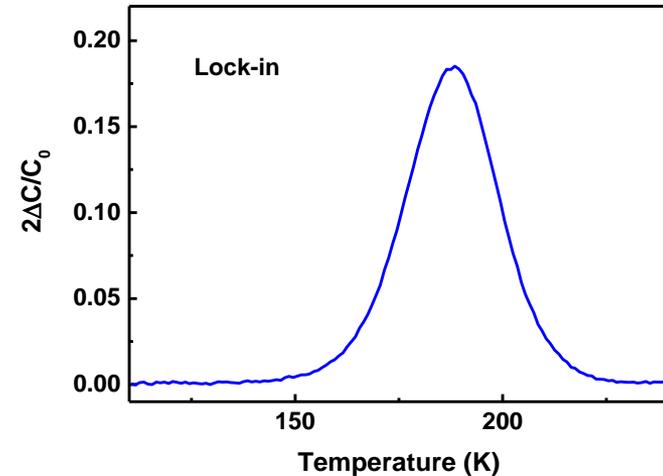
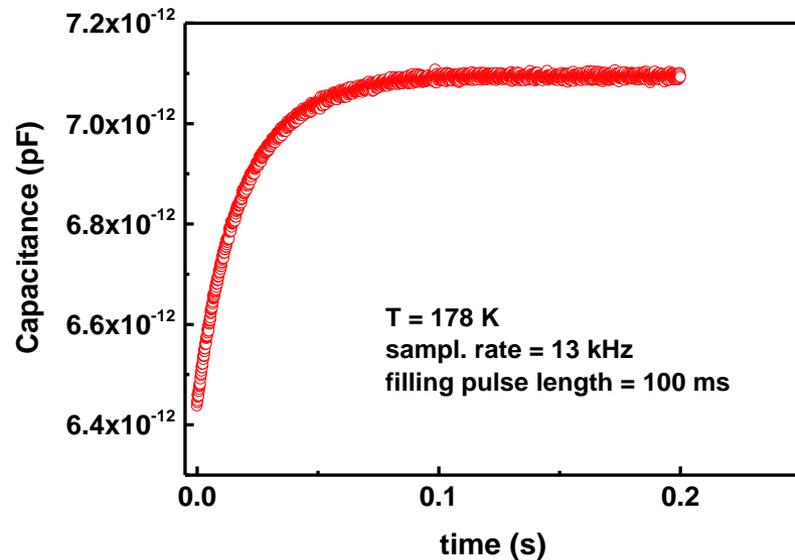
$$w(t - t_p) = \begin{cases} -1 & t_p \leq t < t_p + t_W/2 \\ +1 & t_p + t_W/2 \leq t \leq t_p + t_W \end{cases}$$

- 3) GS4 and following¹

$$w(t - t_p) = \begin{cases} +2 & t_p \leq t < t_p + t_W/4 \\ -26 & t_p + t_W/4 \leq t < t_p + t_W/2 \\ 48 & t_p + t_W/2 \leq t < t_p + 3t_W/4 \\ -24 & t_p + 3t_W/4 \leq t \leq t_p + t_W \end{cases}$$

The choice of the weighting function w

Measurements performed on Pd Schottky contacts to ZnO



- $w_{\text{lock-in}}$ less selective than w_{GS4}
- $w_{\text{lock-in}}$ more stable than w_{GS4}
- Possible presence of false roots and intensity reduction.

Laplace DLTS

Large instrumental broadening in ordinary DLTS spectra

Resolve time constant ratios larger than $\sim 15-12$ (5)

The spectral density of the transient $F(s)$ can be determined by inverting

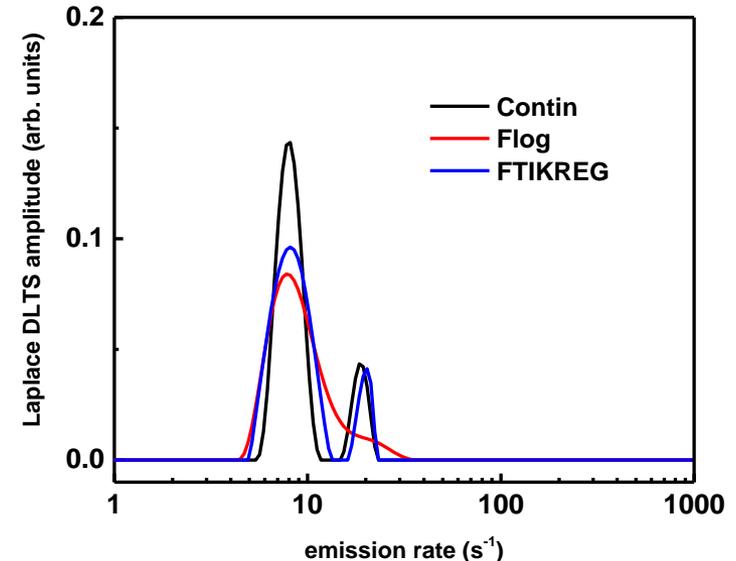
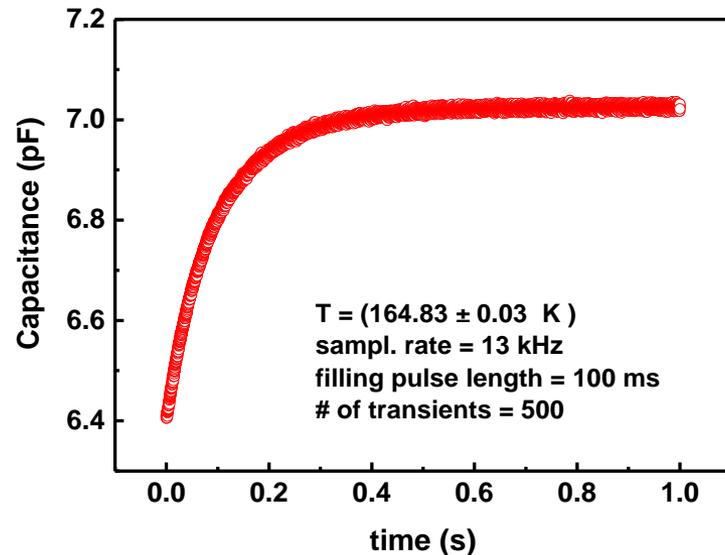
$$\Delta C(t) = \int F(s) \exp(-st) ds$$

Requires isothermal averaging to achieve a "good enough" signal to noise ratio



Possible to study the intrinsic broadening
Resolve time constant ratios larger than ~ 2

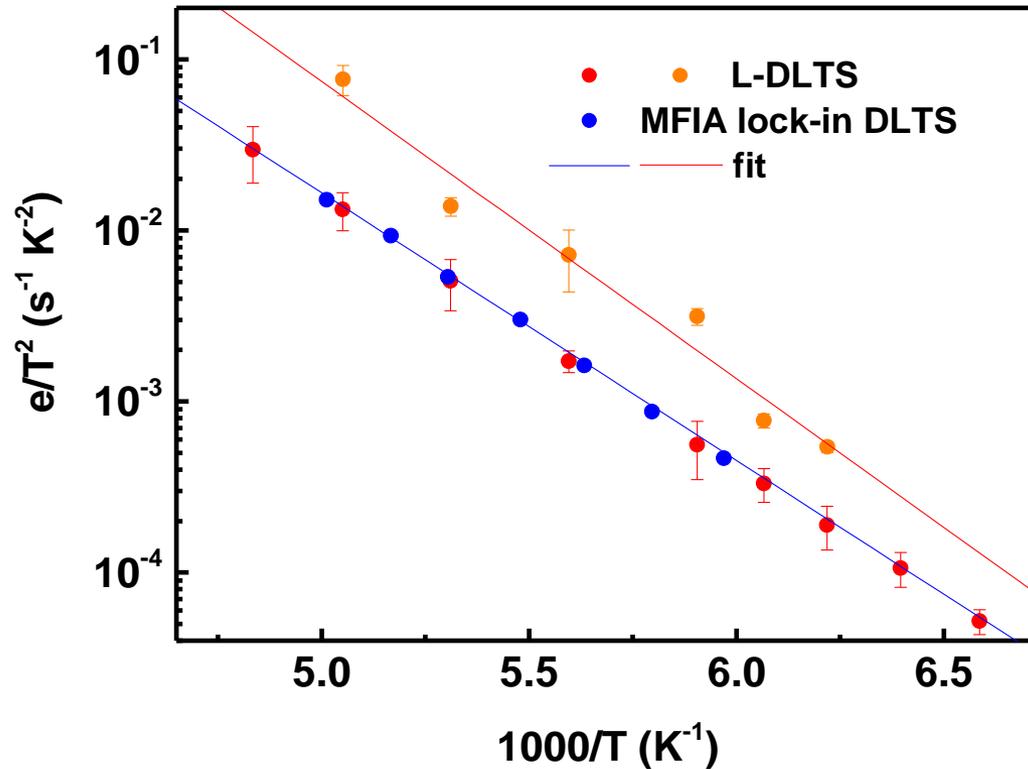
On the analysis of Laplace DLTS transients



Measurements performed on the same sample as previously.

- Several inversion routines can be used.
- Clear evidence for the presence of two components with emission rate ratio ~ 2 .

Defect properties



- From the Arrhenius plot of eT^{-2} vs T^{-1} the defect enthalpy and the apparent capture cross section is extracted:

$$\Delta H \begin{cases} (0.31 \pm 0.1) \text{ eV} \\ \sim 0.34 \text{ eV} \end{cases}$$

$$\sigma_{app} \begin{cases} (1.2 \pm 0.4) \times 10^{-15} \text{ cm}^2 \\ \sim 5 \times 10^{-14} \text{ cm}^2 \end{cases}$$

The E_3/E'_3 levels

$$\Delta H \sim 0.3 \text{ eV}$$

$$\sigma_{app} \sim 10^{-14} - 10^{-16}$$

- Labelled as E_3/E'_3 .
- Present in most samples independently on the growth techniques concentrations up to $\sim 10^{17} \text{ cm}^{-3}$.
- Attributed both to V_O related defects and to Fe/Ni impurities².

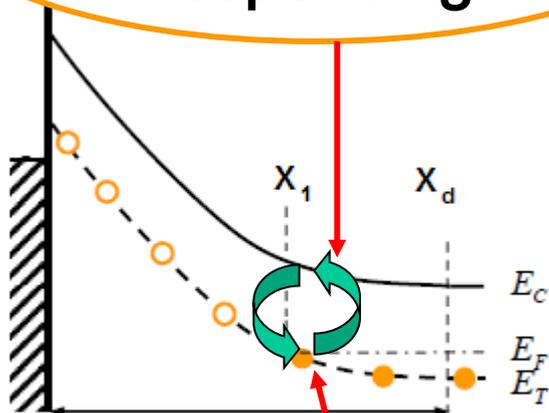
$$e_D \sim 10^5 - 10^6 \text{ s}^{-1} \text{ at } 300\text{K}$$



Important! It can be picked up during C-V measurements at 300 K

TAS principle of the measurement

$f_T \ll e_{D1}(T)$ the centers in x_1 are **responding**



$f_T \gg e_{D1}(T)$ the centers in x_1 are **not responding**

- Fixed reverse bias.
- Capacitance and conductance measured with probing frequency f_T ($\omega_T = 2\pi f_T$).
- Temperature is scanned.
- Only majority carriers involved.
- Responding defects at the edge of the depletion region i.e. negligible electric field effects.

TAS spectra (not formal)

- Pure capacitance = Schottky contact: Q and V in phase
- Capacitance for a Schottky contact/junction with defects:

$$Q = \text{Re}(Q_0 e^{j(\omega t - \varphi(T))}) = Q_0 \cos(\omega t - \varphi(T)) = \\ = Q_0 (\cos \omega t \cos \varphi(T) + \sin \omega t \sin \varphi(T))$$

Delayed defects
response

By lowering the temperature it is observed:

- 1) a capacitance drop
- 2) a conductance increase.

TAS spectra (more formal)

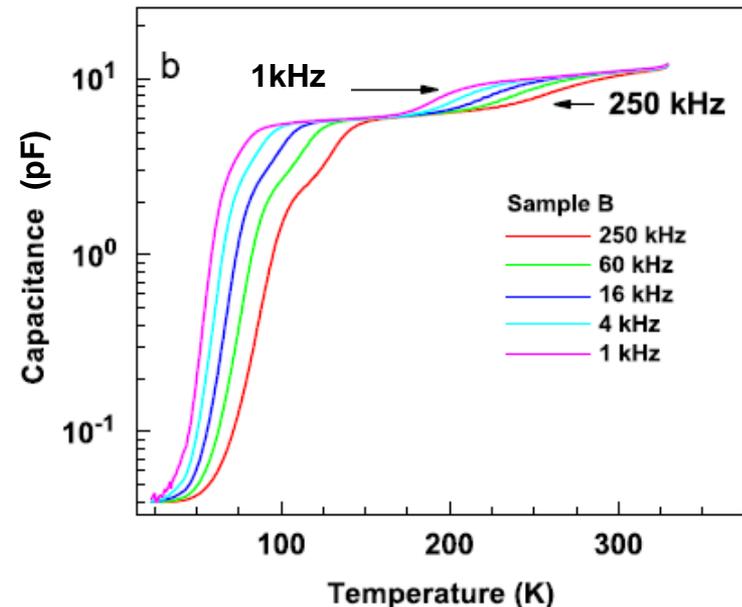
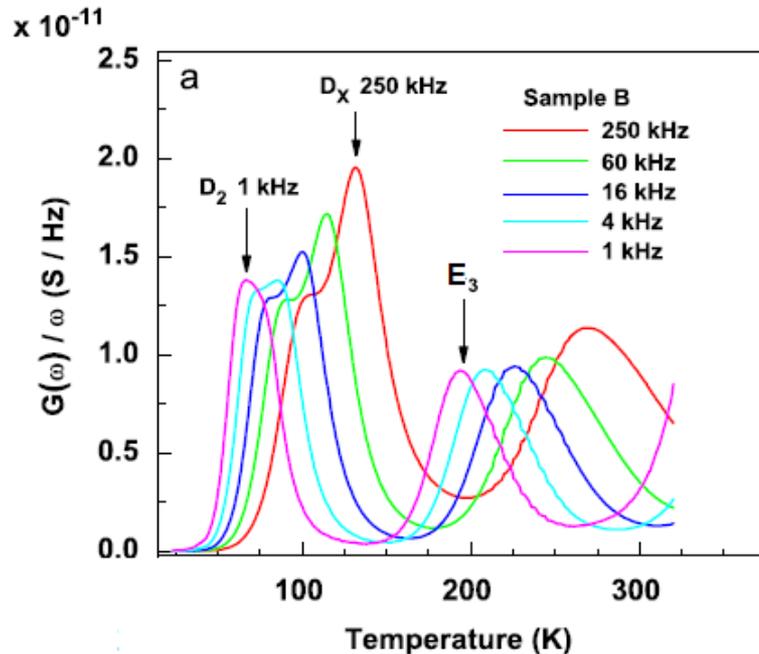
$$\Delta C = C_{HT} - C_{LT} \propto \frac{N_T}{N_D} \frac{(1-x_1/x_d)}{(1-(x_1 N_T)/(x_d N_D))}$$

$$\frac{G(\omega_T)}{\omega_T} = \Delta C \frac{\frac{\omega_0}{\omega_T}}{1 + \left(\frac{\omega_0}{\omega_T}\right)^2}$$

$$\frac{\omega_0}{T_{max}^2} \propto \exp\left(\frac{-\Delta H}{k_B T}\right)$$

- Cantilever effect i.e. $\Delta C \rightarrow 0$ for increasing reverse voltages.
- No limitation on the N_T/N_D ratio.
- The probing frequencies have to be comparable to the emission rate ($\gtrsim 1/\pi$ times).

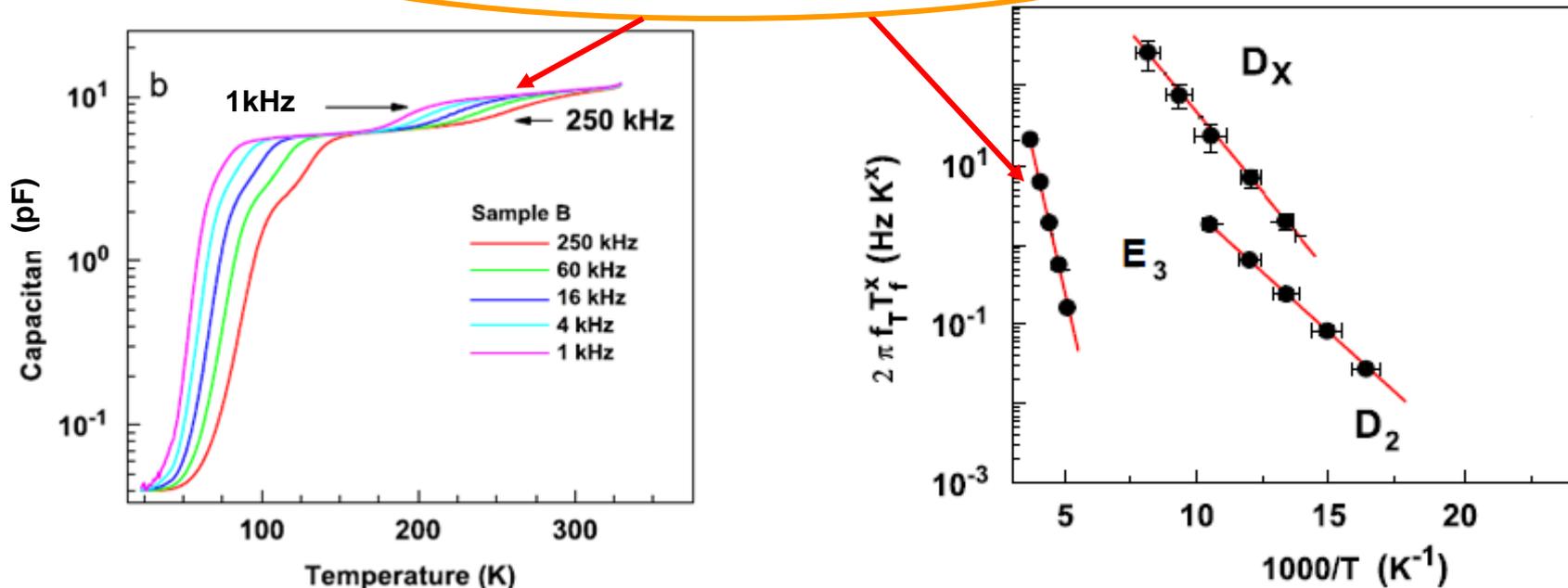
On the analysis of TAS spectra: an example (1)



- Presence of leaking mechanisms may provide an increasing background in the conductance plot.
- Cantilever effect measurements particularly sensitive to the interfacial states.

On the analysis of TAS spectra: an example (2)

E_3 is responding at 250 kHz

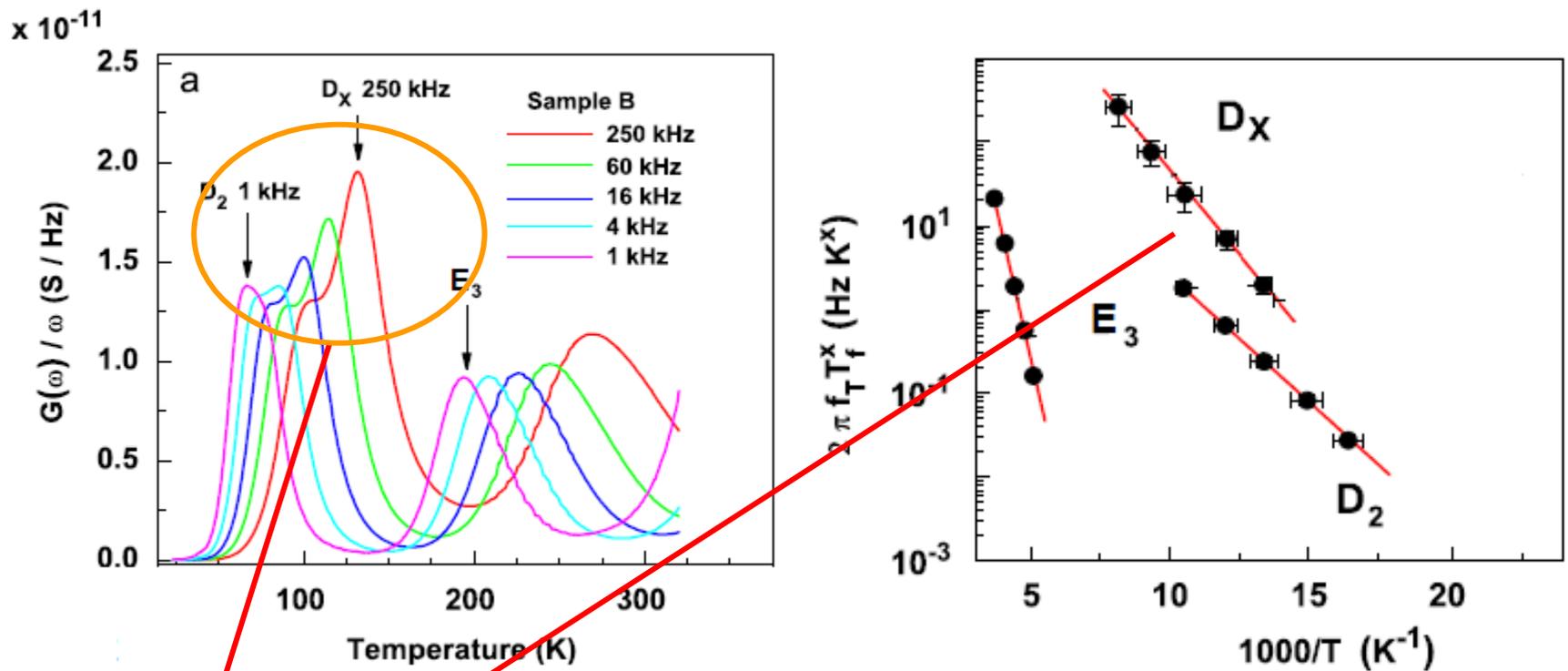


- From the Arrhenius plot of $\omega_0 T^{-2}$ vs T^{-1} the defect enthalpy and apparent capture cross section is extracted (N.B. $\omega_0 \neq 2e$ in the general case).

$$\Delta H = (0.29 \pm 0.03) \text{ eV}$$

$$\sigma_{app} = (6 \pm 3) \times 10^{-16} \text{ cm}^{-2}$$

On the analysis of TAS spectra: an example (3)

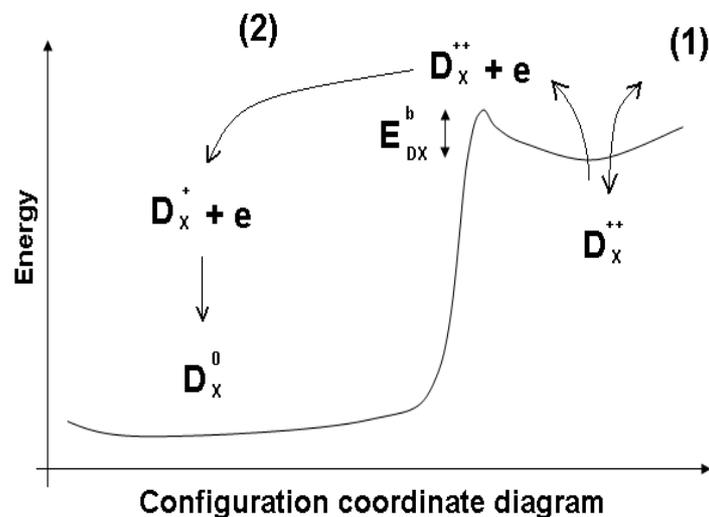


- The D_X temperature dependence points to a thermally activated process.
- Ordinary DLTS measurements do not reveal any signature corresponding to D_X .

The proposed model for D_x

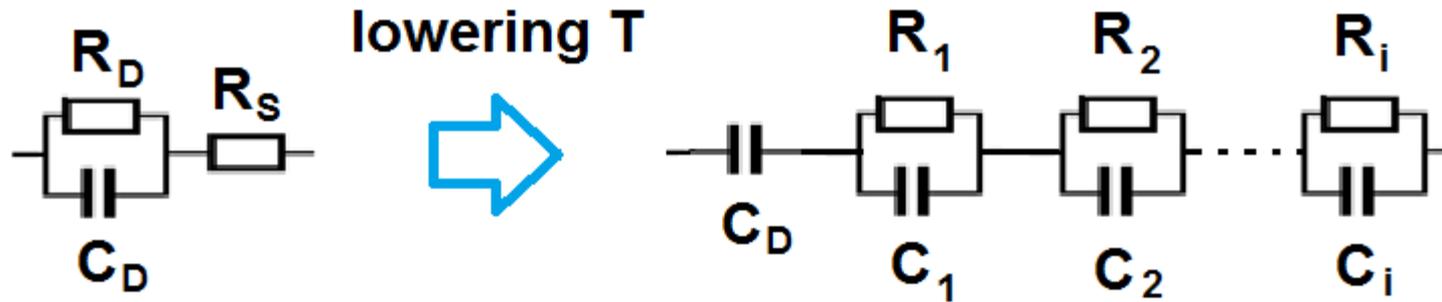
Two processes can occur:

- 1) D_x^{++} level probing \rightarrow TAS peak.
- 2) Electron capture ($D_x^{++} \rightarrow D_x^{++} + e$) followed by the atomic reconfiguration and the capture of a second electron ($D_x^+ + e \rightarrow D_x^0$) \rightarrow ordinary DLTS.



- D_x negative-U defect possibly V_O .
- The high probing frequency permits to detect defects that are changing their configuration when charged (defects not so easy to detect with DLTS/L-DLTS).

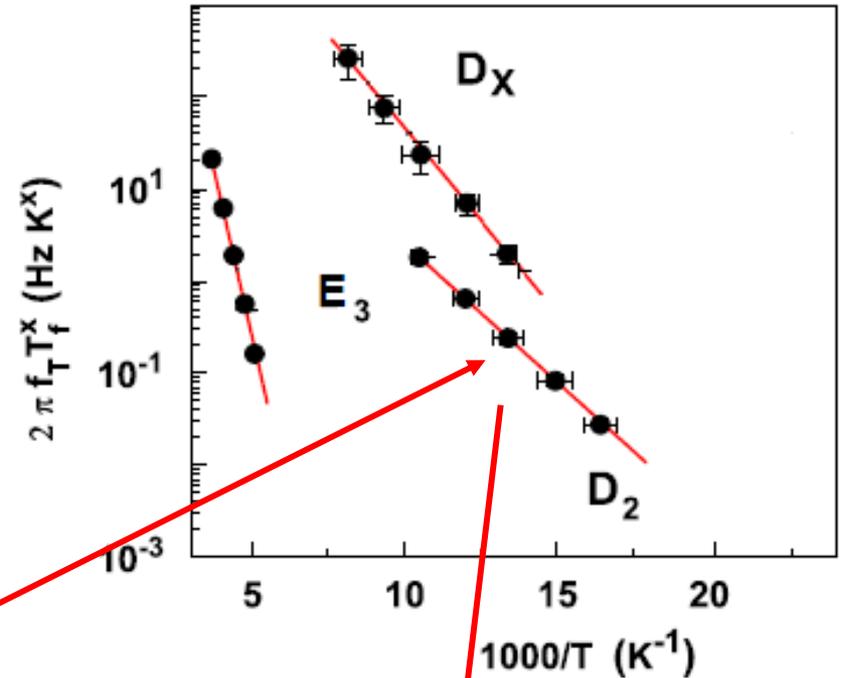
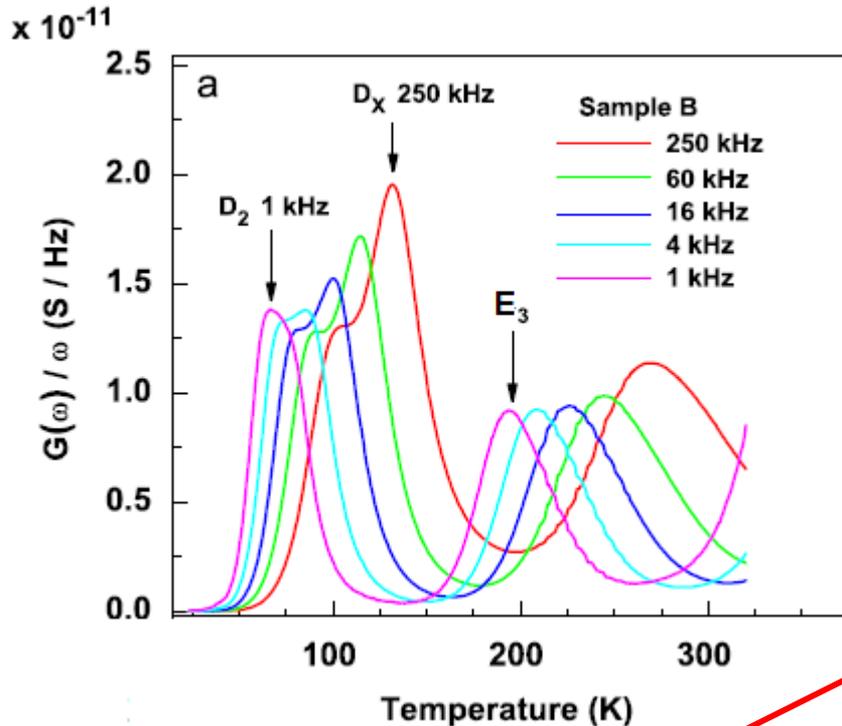
TAS spectra (freezing-out)



Similarly to ordinary TAS peaks the $\frac{G(\omega_T)}{\omega_T}$ freeze-out peak corresponds to $\frac{\Delta C}{2}$ and occurs for $C_D R_{tot} \omega_T = 1$

$$\Rightarrow \frac{2\pi f_T}{\mu(T) T^{\frac{3}{2}_{\max}}} \propto \exp\left(\frac{-\Delta H}{k_B T}\right)$$

TAS: main donor parameters extractions



- If $\mu(T)$ in the freezing-out temperature range is known ΔH can be evaluated.

$$\mu(T) \propto T^{\frac{3}{2}}$$

$$E_{D2} = (50 \pm 10) \text{ meV}$$

DLTS

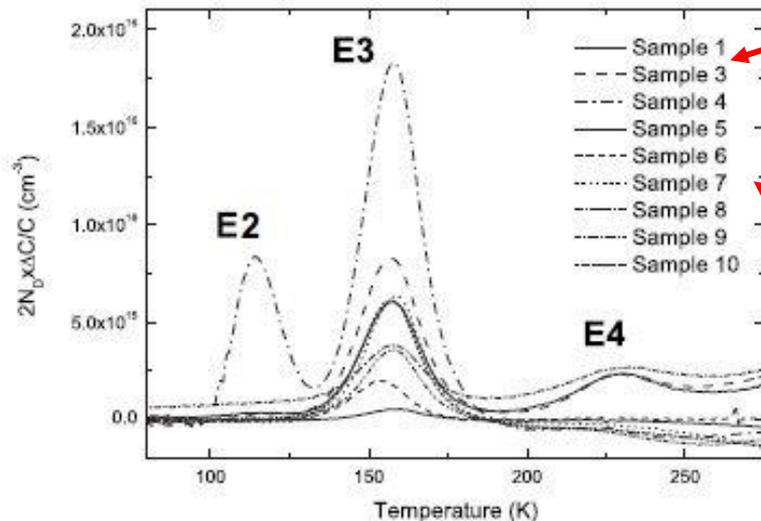
- Volume measurement → large reverse biasing preferred → good rectifying junction.
- Dilution limit i.e. $N_D \gg N_T$.
- Presence of electric field (Poole-Frenkel effect).
- Possible minority carriers injection.
- Rate window/transient time window limiting the range of investigated emission rates.

TAS

- $E_T - E_F$ cross region response → small reverse biasing preferred → not so good rectifying junction required.
- No dilution limit. No minority carriers injection. Negligible electric field in the probed region.
- Probing signal determining the investigated emission rates. Possible to detect defects with changing configurations.

How to establish the nature of the defect

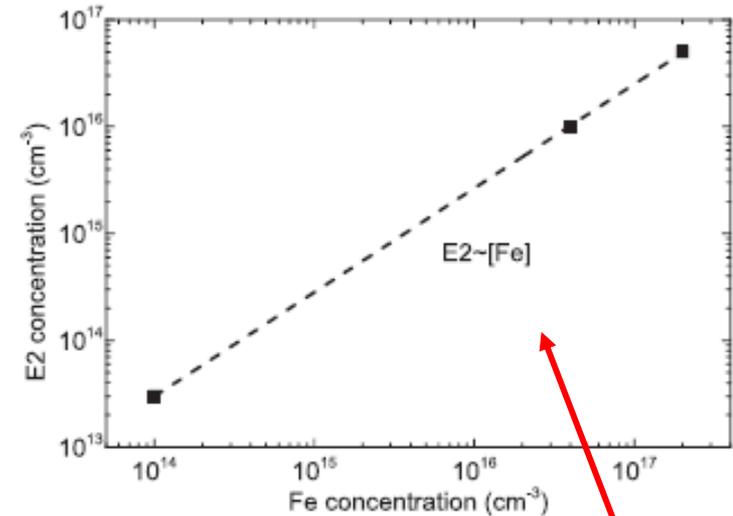
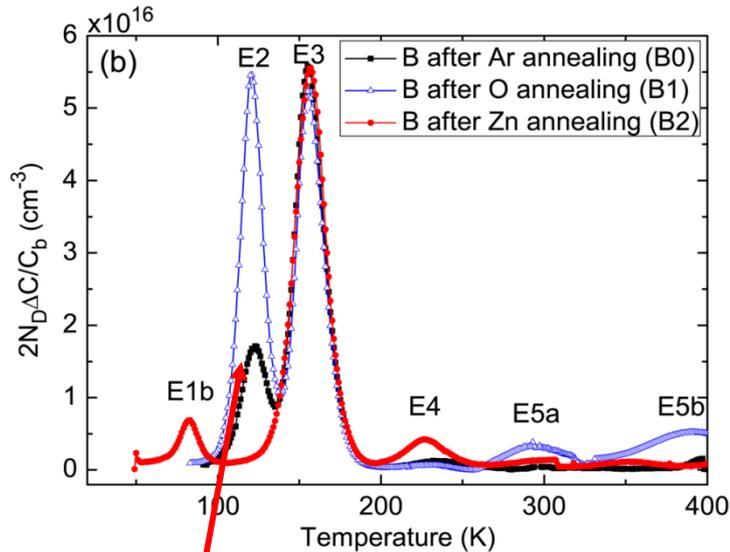
- DLTS spectra is providing: σ_{app} ; ΔH ; N_T
- Comparative studies are required: annealing, implantation, electron irradiation can be used to alter N_T in establishing the chemical nature of the defect.



1,2 References

Annealed at 1100 - 1500 °C
for 1 h in air

Example 1: an annealing study on ZnO



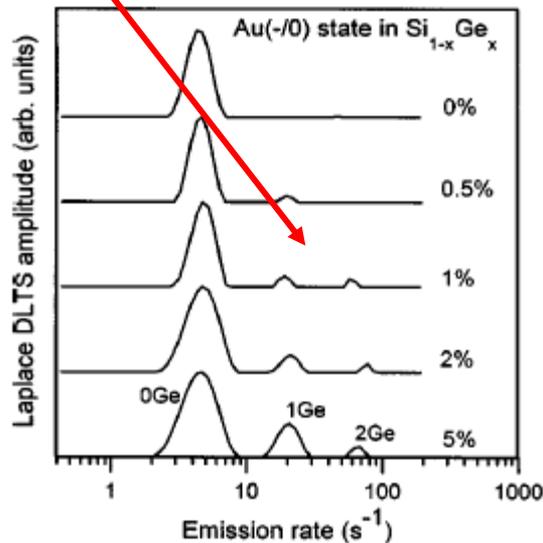
Increases with annealing in O_2 at $1100\text{ }^\circ\text{C}$

E_2 accounts for $\sim 30\%$ of the total Fe concentration measured by SIMS

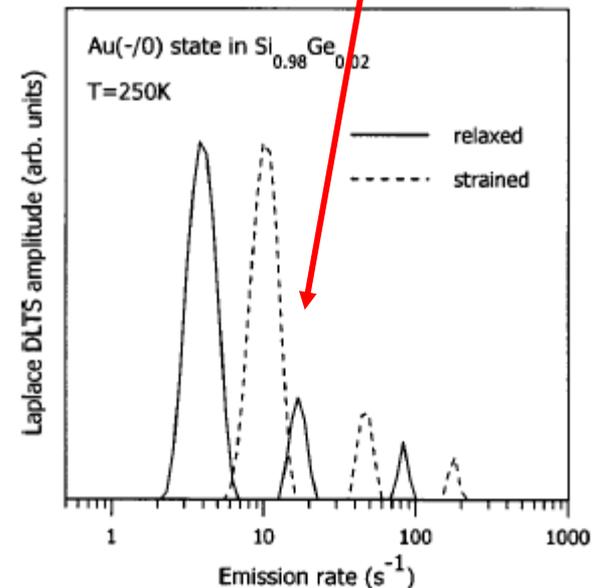
- E_2 involves Fe in a configuration enhanced by O-rich conditions such as Fe on Zn site

An example: Laplace DLTS on SiGe

Effect of the local environment on the Au acceptor in SiGe



Effect of the strain on the Au acceptor in SiGe



Laplace DLTS can be thought as a truly spectroscopic technique



Literature (books)

- 1) S. M. Sze and M. K. Lee, **Semiconductor Devices**, John Wiley & Sons (2012).
- 2) E.H. Rhoderick, R.H. Williams, **Metal-Semiconductor Contacts**, Oxford University Press (1988).
- 3) P. Blood, J.W. Orton **The Electrical Characterization of Semiconductors: Majority Carriers and Electron States**, Academic Press, London (1992).



Literature (articles)

Alternative method to evaluate the series resistance

- 1) J. H. Werner, Appl. Phys. A **47**, 291 (1998)

DLTS/L-DLTS literature/links:

- 1) L. Dobaczewski, A. R. Peaker, and K. B. Nielsen, J. Appl. Phys. **96**, 4689 (2004)
- 2) http://info.ifpan.edu.pl/Dodatki/WordPress/laplacedlts/?page_id=9#TPU
- 3) Zurich Instruments Application Note

TAS literature:

- 1) J. L. Pautrat, B. Katircioglu, N. Magnea, D. Bensahel, J. C. Phister and L. Revoil, Solid State Electronics **23**, 1159 (1980)
- 2) R. Schifano, E. V. Monakhov, B. G. Svensson, W. Mtangi, P. Janse van Rensburg, and F. D. Auret, Physica B **404**, 4344 (2009)