EXPERIMENTAL OBSERVATION OF MOVING DISCRETE BREATHERS IN GERMANIUM

MINISTERIO
DE CIENCIA
E INNOVACIÓN

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Nonlinear localized travelling excitations in crystals.
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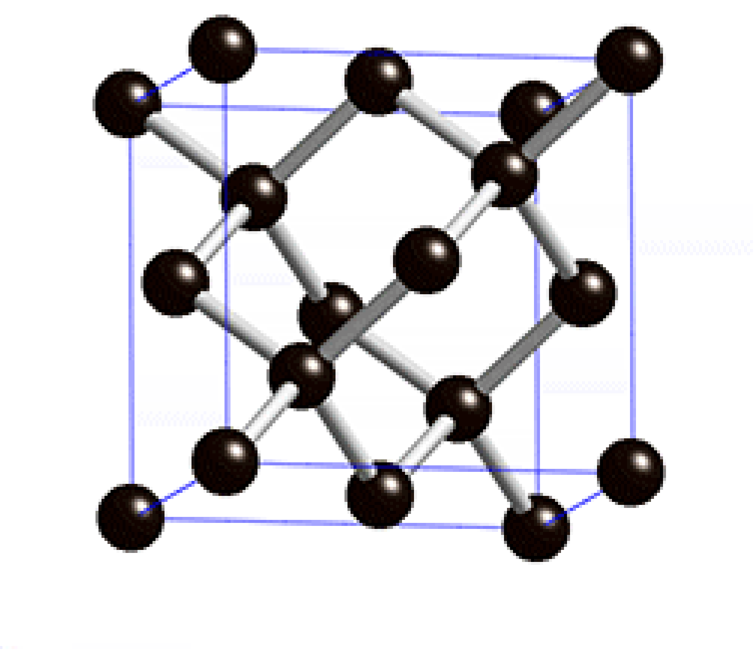
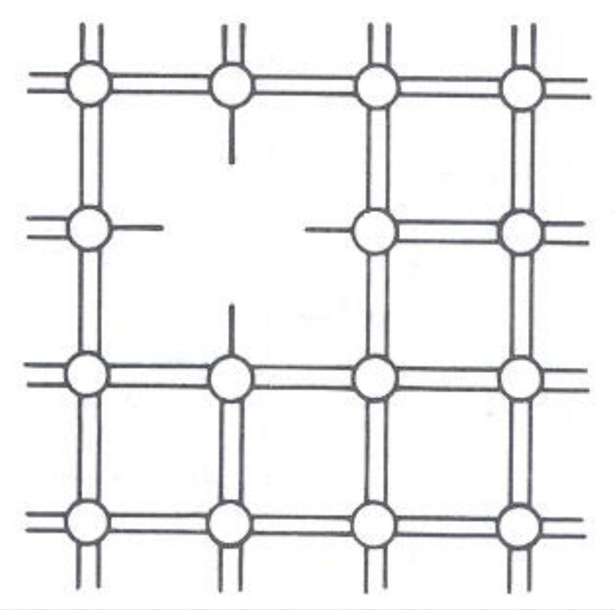
Germanium

- Unlikely structure for moving discrete breathers

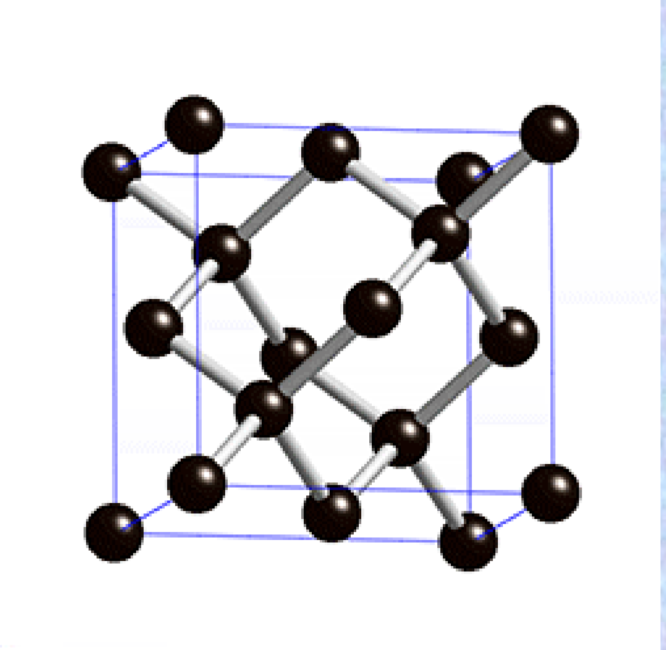




Outline

We believe that there are moving discrete breathers in Ge

- What property allows for their detection? Defect annealing
- What technique we use to detect them: DLTS
- How efficient DB with respect to phonons for annealing?
- What characteristics about breathers in Ge we can estimate?



Germanium

At room temperature (RT, 300 K) the size of the band gap is 0.66 eV while increasing with decreasing temperature to 0.74 eV at a temperature of a few K

Relative effective masses (density of states)

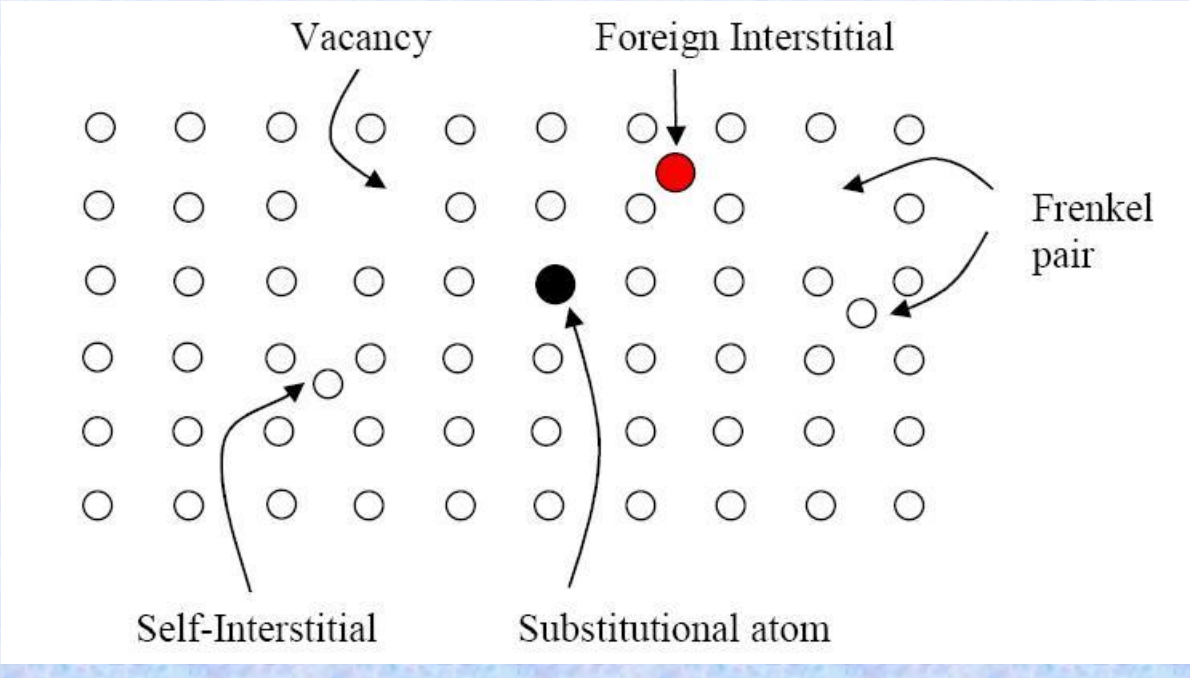
	Si	Ge
Electron	1.08	0.55
Hole	0.56	0.37

Typical (low doping) values

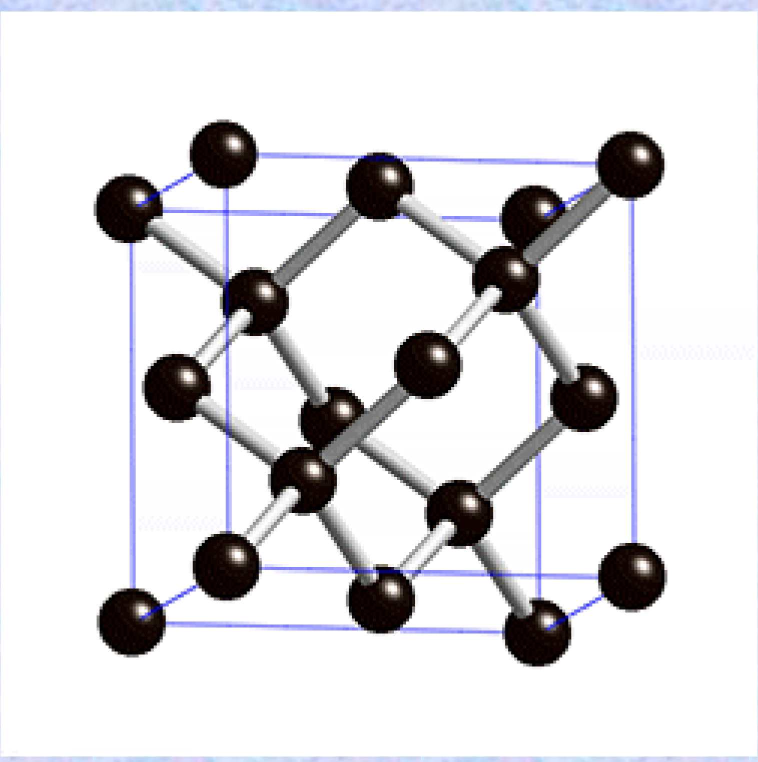
	Si	Ge	
Electron mobility (cm^2/Vs)		1350	3900
Hole mobility (cm^2/Vs)	480	1900	

Defects in germanium

- Can be produced by irradiation
- Of technological interest

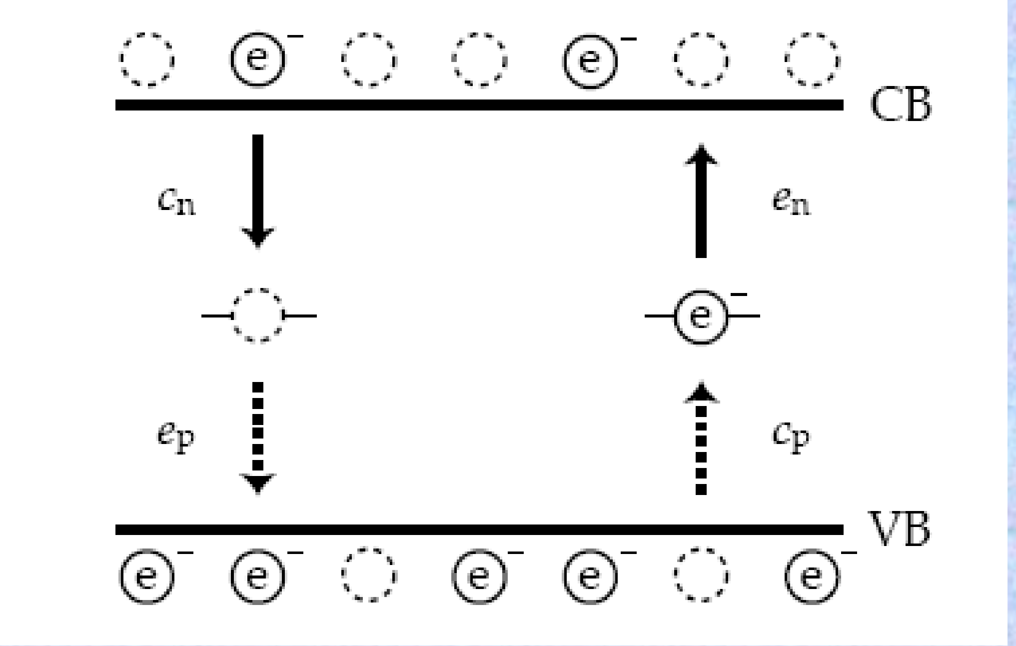


Some complex defects in germanium



- Di-vacancy V-V
- Tri-vacancy V_3, Tetra-vacancy V_4
- Vacancy-Hydrogen VH_n
- I_2, I_3, …
- A center:
  Foreign interstitial 0-Vacancy
- E center
  Substitucional atom-Vacancy
  Sb doped Ge: Sb-V

Defect as electron and hole traps



Dynamics of an energy state.

The solid arrows : electron capture/emission

Dashed arrows: hole capture/emission.

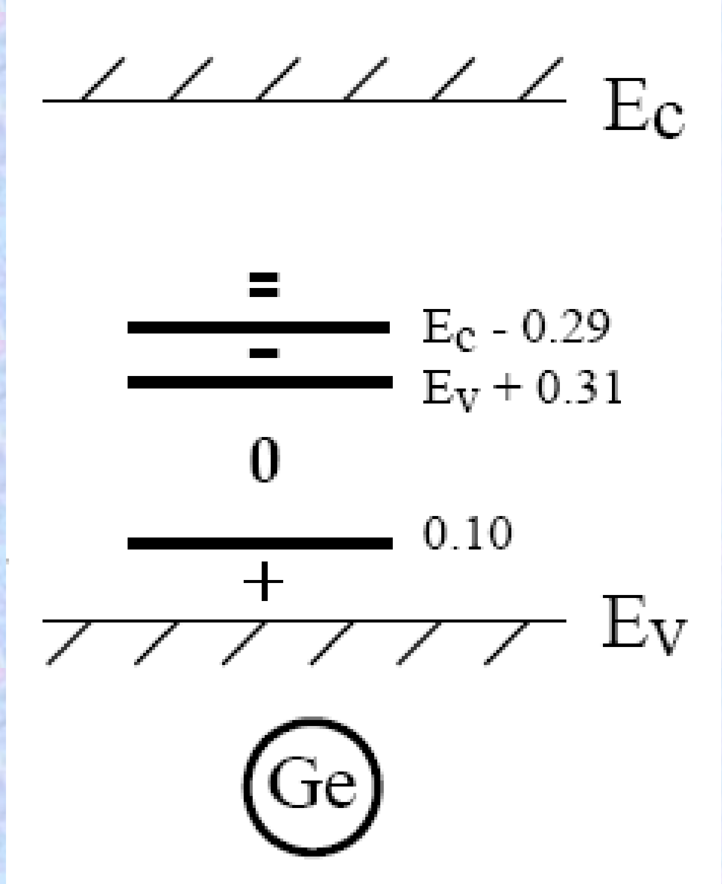
Empty level. defect can
-Capture an electron
from the CB (c_n)

-Emit a hole
to the VB (e_p)

Defect populated by an electron can :
-Emit an electron
to the CB (e_n)

- Capture a hole
from the VB (c_p)

Electron and hole traps



- Defects have aceptor or donor levels

- Deep levels: far from the nearest band (>0.1 eV).

- Ec-Ev=0.67 eV

- Electron trap:

  n-type $E_{0.29}$
- Hole trap

  p-type $H_{0.10}$

Capture and emision rate of an electron trap

Capture rate $c_n = \sigma_n \langle v_n \rangle n$

Emission rate $e_n = \sigma_n \langle v_n \rangle N_c \exp(-\frac{E_T}{kT}) = \sigma_n \gamma_n T^2 \exp(-\frac{E_T}{kT})$

Activation energy for electron emission: $E_T = E_C - E_t$

γ_n depends on fundamental constants and m_e^*

Signature of a defect: E_T , σ_n

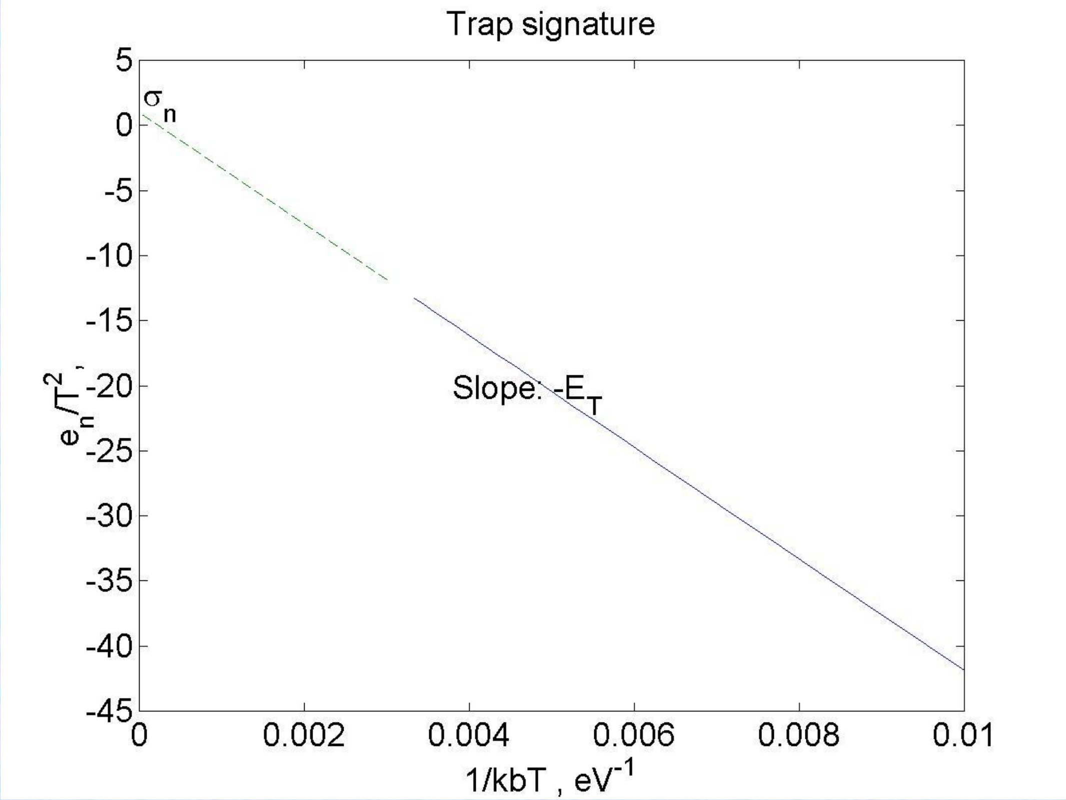
Number of defects or traps: N_T

Other type of parameters:

- Energy barrier for annealing: E_0
- Temperature of annealing:

Capture and emision rate of an electron trap

$$e_n = \sigma_n \langle v_n \rangle N_c \exp(-\frac{E_T}{kT}) = \sigma_n \gamma_n T^2 \exp(-\frac{E_T}{kT})$$



DLTS: Deep Level Transient Spectroscopy

Objective: find the trap parameters and concentration
Magnitude measured: electron lifetime in a trap:at different temperatures $\tau_n = 1/e_n \;;\; \tau_n = \tau_n(T)$

Needs a depletion layer as in p-n junction or Schottky diode under reverse bias

Procedure: Fill all the trap levels and measures the capacitance at two different times as traps emit electrons and discharge.

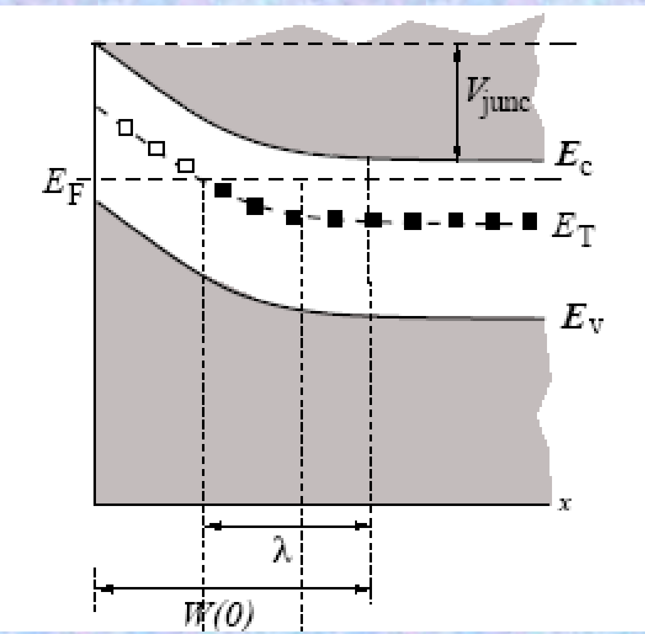
$$\Delta C = C(t_1) - C(t_2)$$

DLTS signal or transient:

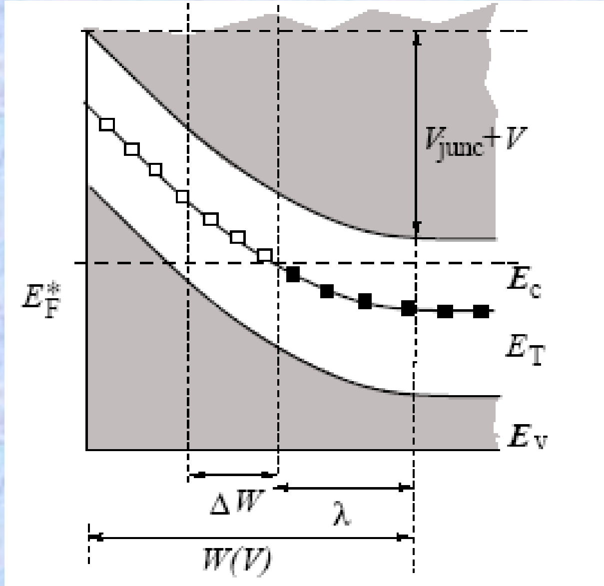
Repeats the procedure as the temperature changes. $\Delta C = \Delta C(T)$

DLTS: Deep Level Transient Spectroscopy

p+-n junction   or Schotty diode (metal-semiconductor)



Zero bias



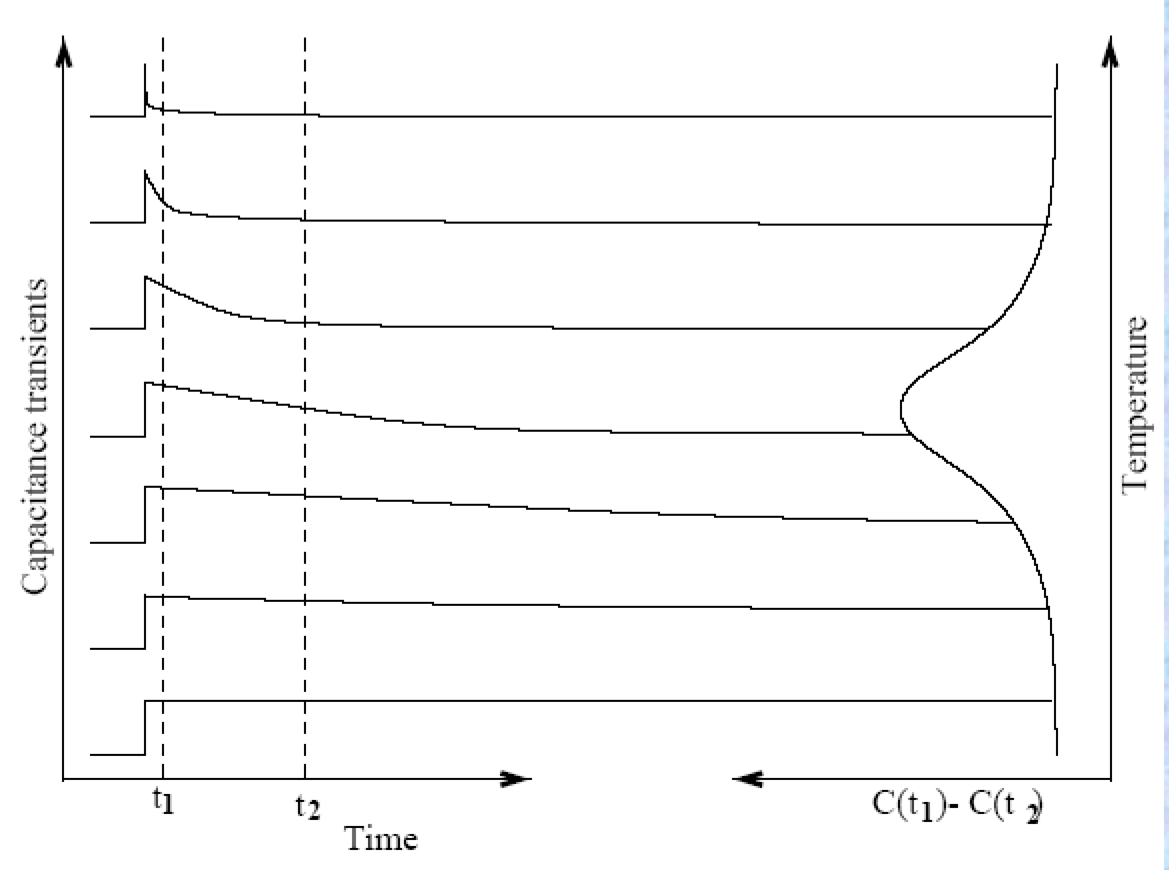
Reverse bias

ΔW: depletion region.

Then: biasing pulse fills the depletion region with electrons filling the traps, which subsequently emit

DLTS: Deep Level Transient Spectroscopy

Capacitance transients:



Zero bias

$$C(t) = C_0 \exp(-t/\tau_n)$$

$$\tau_n = 1/e_n$$

Life time of an electron in the trap decreases with T

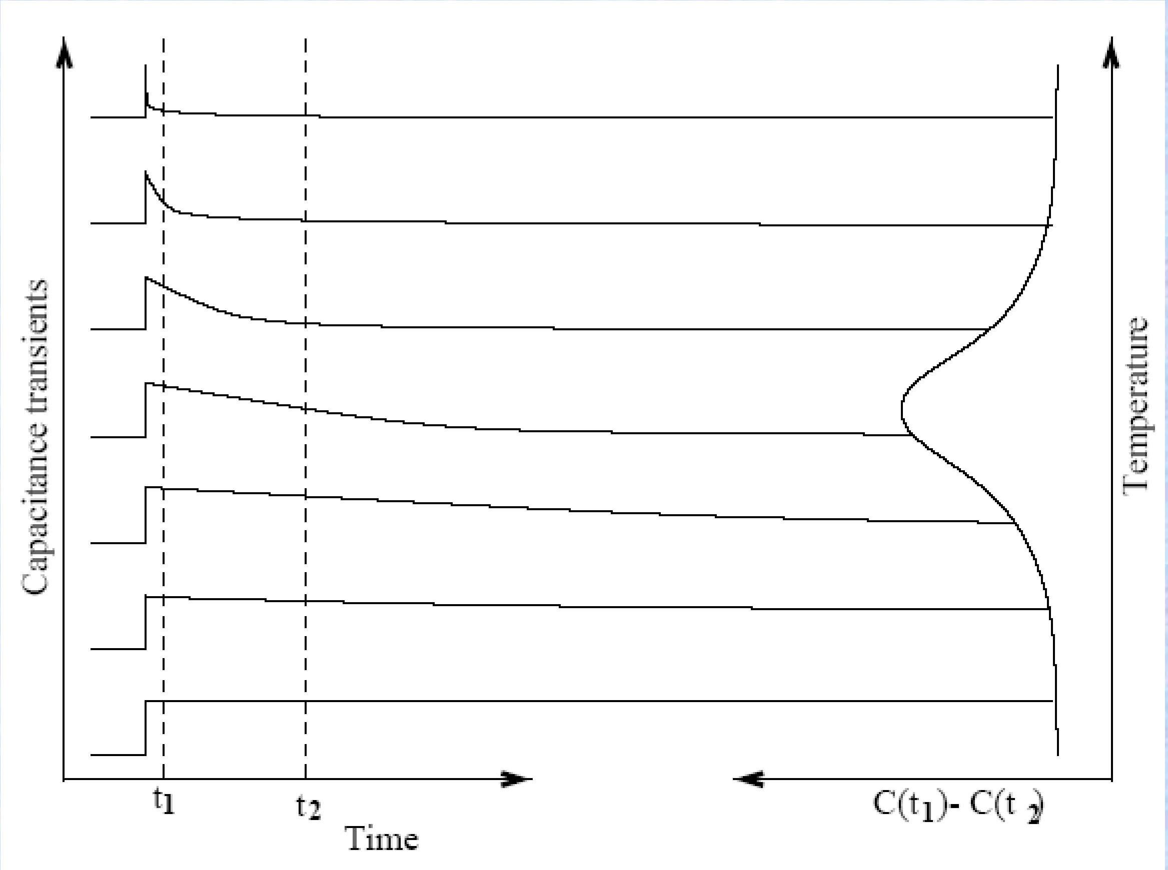
DLTS: Rate window

$$\Delta C(\tau) = C_0(\exp(-t_1/\tau) - \exp(-t_2/\tau))$$

has a maximum at

$$RW = 1/\tau_{\max} =$$

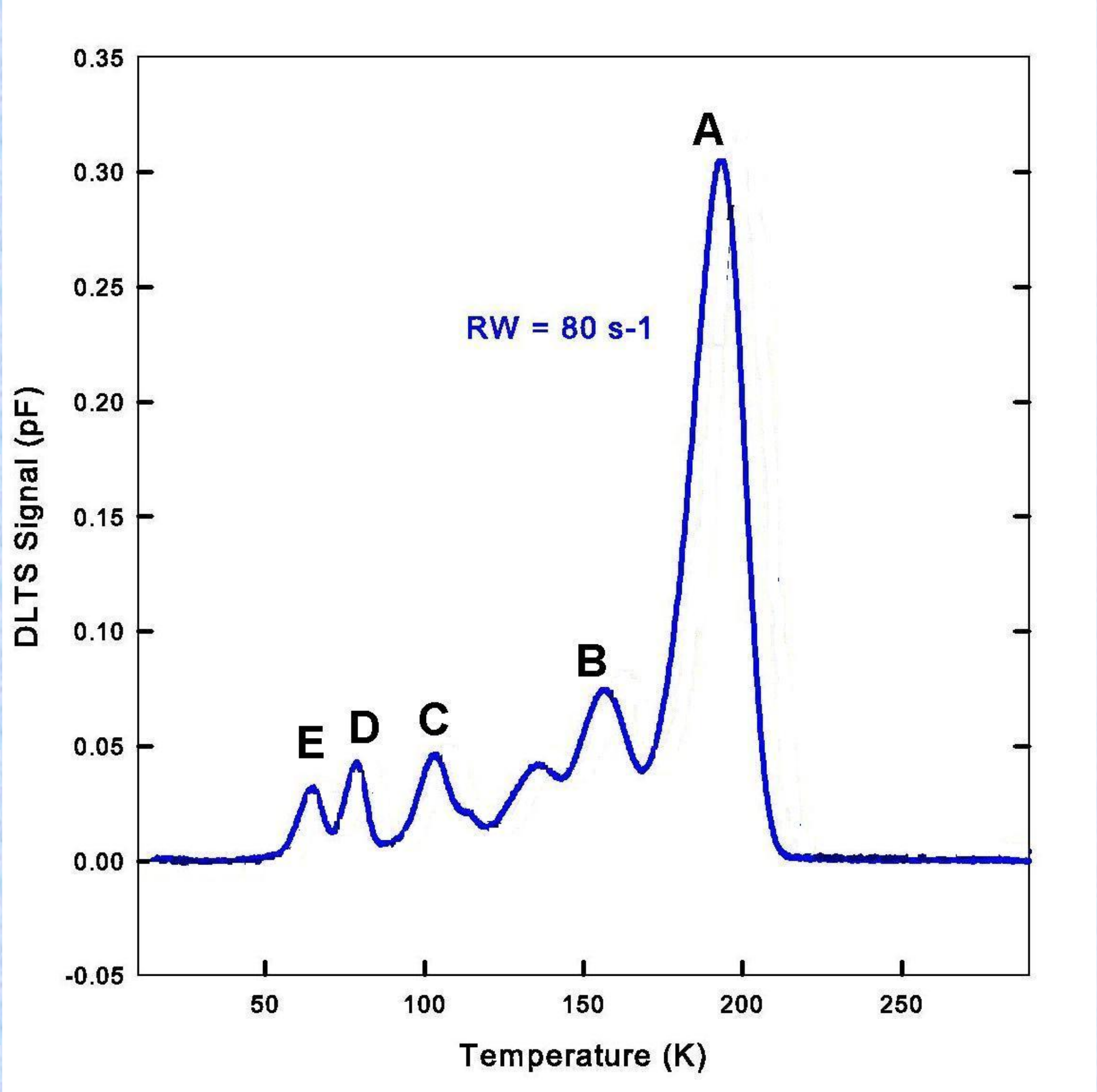
$$\ln(t_1/t_2)/(t_1-t_2)$$



Typical RW are
80 s^{-1} and 200 s^{-1}

When the emission rate $e_n(T)$=RW there is a maximum at ΔC= ΔC(T)

DLTS: Example



Defect A:

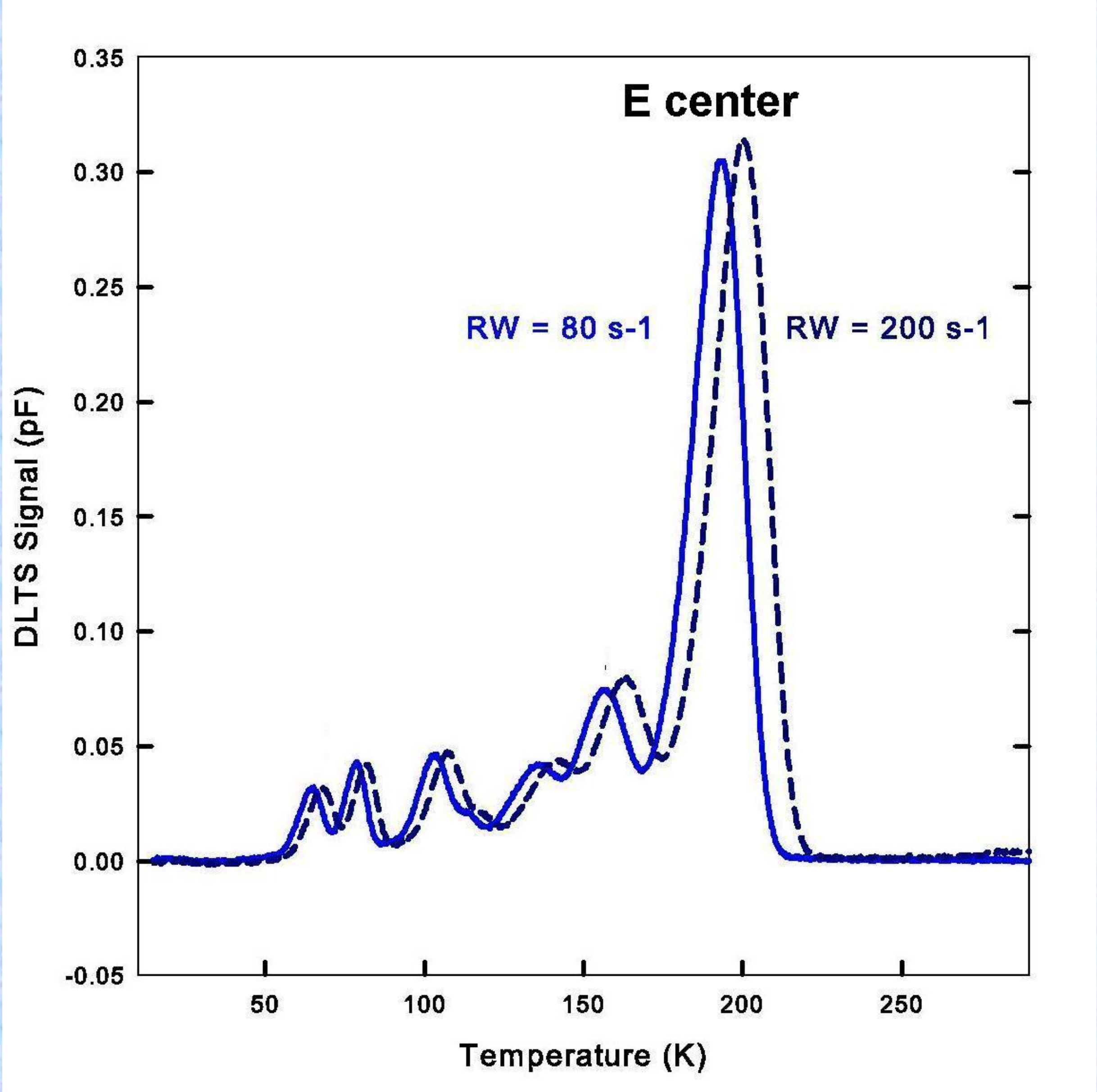
$$RW_1 = 80s^{-1} = e_n(T_A)$$

Defect B:

$$RW_1 = 80s^{-1} = e_n(T_B)$$

Defect C …..

DLTS: Example, two RW: Defect E center



$$RW_1 = 80s^{-1} = e_n(T_1) =$$

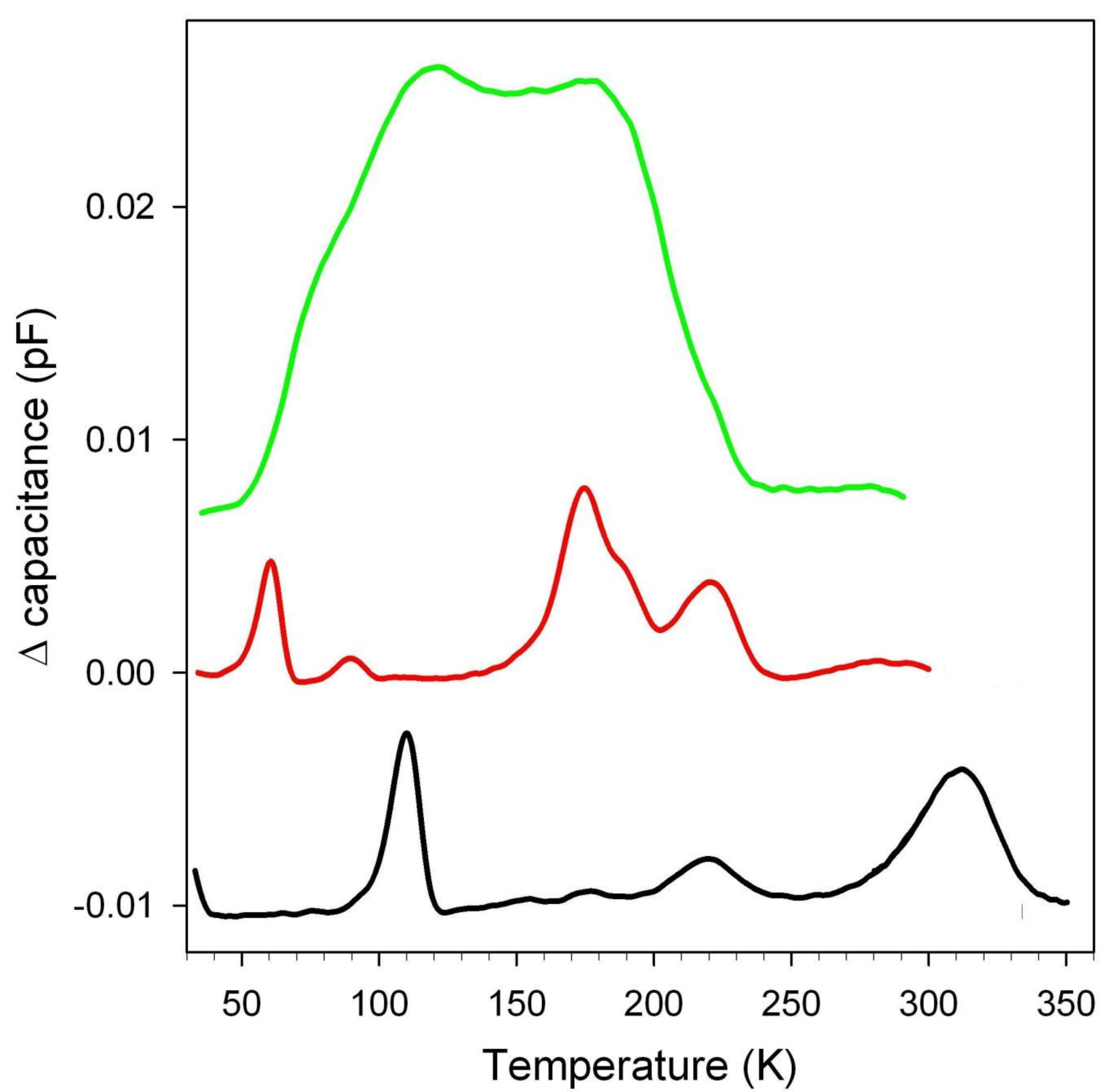
$$\sigma_n \gamma_n T_1^2 \exp(-\frac{E_T}{kT_1})$$

$$RW_2 = 200s^{-1} = e_n(T_2) =$$

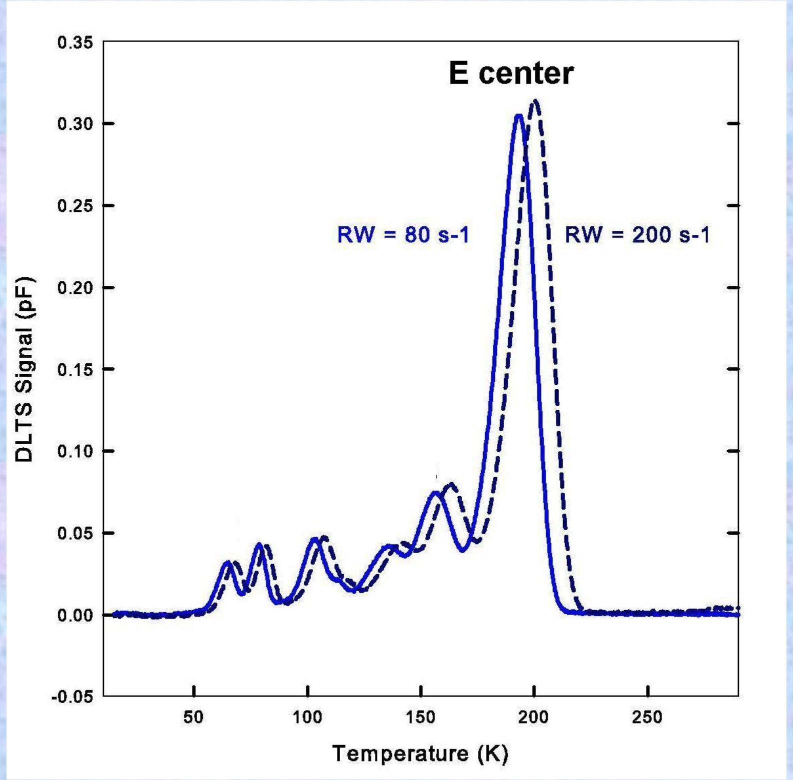
$$\sigma_n \gamma_n T_2^2 \exp(-\frac{E_T}{kT_2})$$

σ_n and E_T can be determined

DLTS: Two many defects!



Number of traps for n-type semiconductor:



N_D :concentration of donors

$$\frac{\Delta C}{C_0} = \frac{N_t}{2N_D}$$

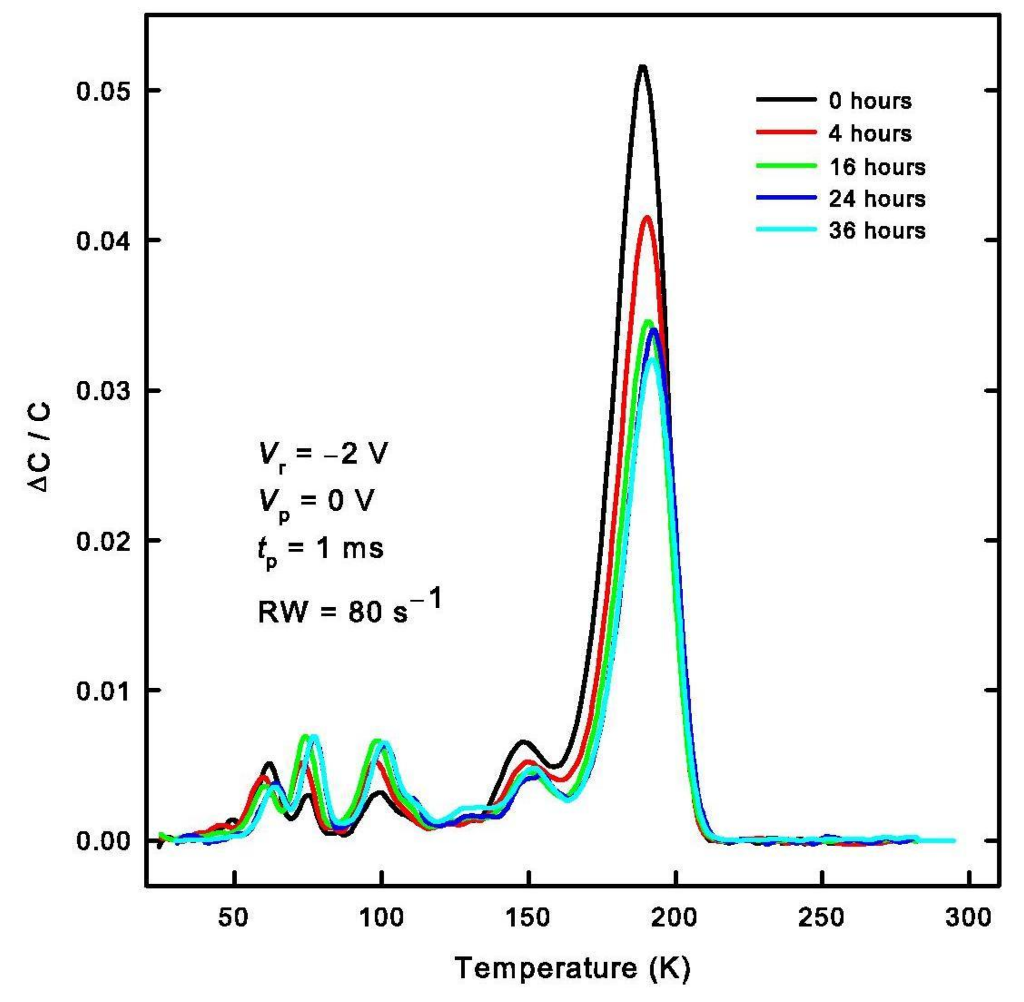
The number of traps N_t can be determined

The depletion layer with W increases with the bias potential:

The profile $N_t(x)$ can be obtained

Annealing: isochronal: same time, different temperatures
Time: annealing with time, same temperature.
Annealing temperature and activation energy E_0 can be obtained

Annealing at room temperature



$$\frac{dN_t}{dt} = -k(T)N_t$$

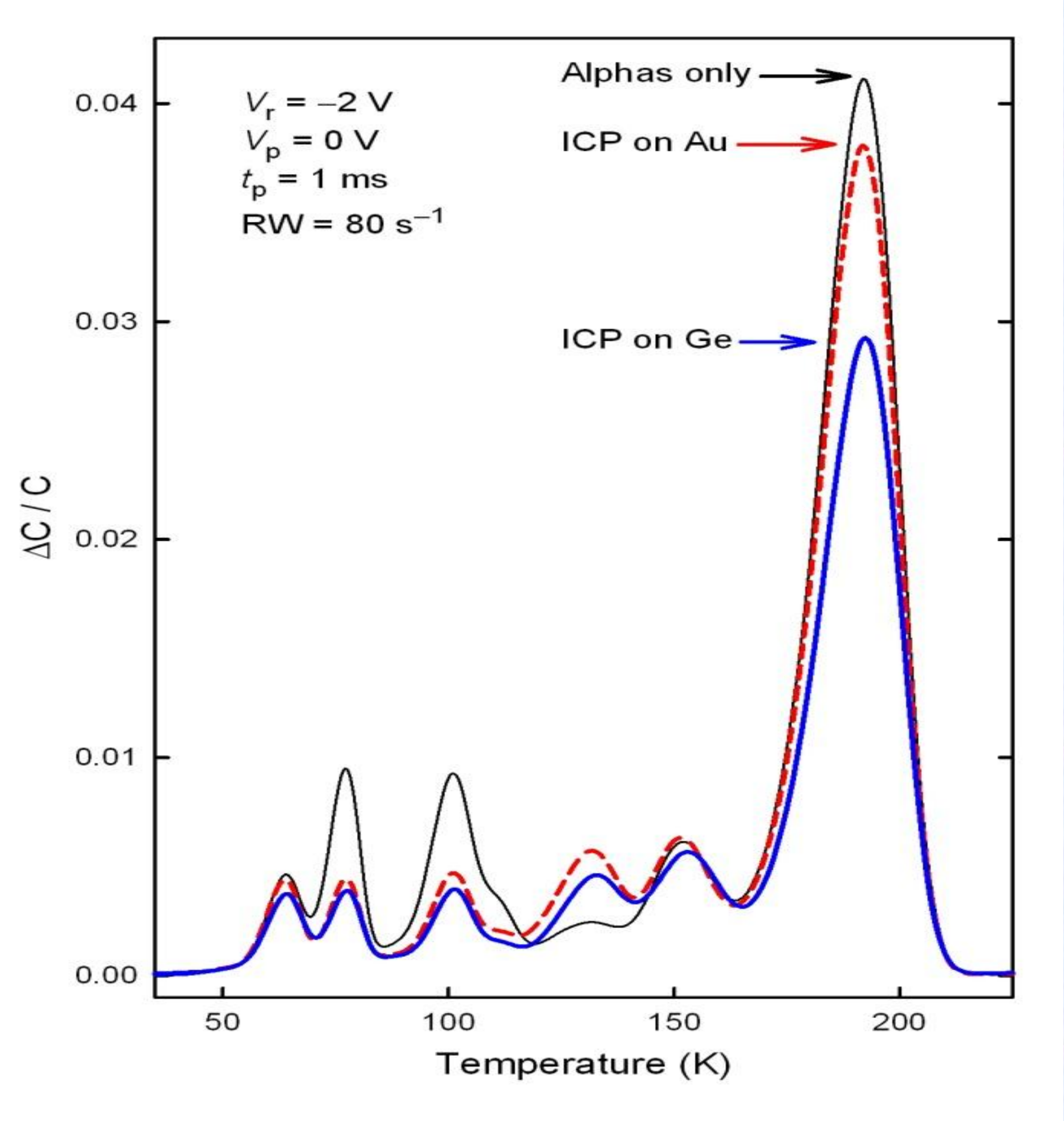
$$k(T)\ \alpha\ \exp\left(-\frac{E_0}{k_B T}\right)$$

Annealing **rate constant** ***k(T)*** can be determined

Isochronal annealing: same time, different temperatures

Annealing activation energy E_0 can be determined

Our basic experiment: 4 eV ICP plasma annealing



1.-Sb doped Ge is damage with 5 MeV alpha particles

2.- Rest 24 hours

3.-Au diode is evaporated in half the sample (half A)

4.- DLST in A
(black, alphas only)
5.-ICP in A and B

6.- Au diode in B

7.- DLTS in A (red-dashed)
(red, ICP on Au)

8.- DLTS in B
(blue, ICP on Ge)

Our basic experiment: Facts

1.-Sb concentration: $1.3\cdot10^{15}$ cm^{-3} (n_i= $2.4\cdot10^{13}$ cm^{-3}) ; 1 Sb per 10^8 Ge

2.- Metal (Au) thickness: 25nm

3.- After ICP on Ge the E center concentration drops 29% from N_T= $1.07\cdot10^{14}$ cm^{-3}

4.- If ICP is done on Au, the E center reduction is smaller, but exists.

5.- ICP is done for 30’ in intervals to prevent heating

6.- Defect annealing occurs up to 2600 nm or 4600 lattice units

7.- If the plasma energy is increased the effect is smaller

8.- Thermal annealing has to be done at 150 C to obtain a similar effect

Our hypothesis: Ar ions impacting on Ge produce Discrete Breathers, which travel through Ge and anneal the defects. Why?

1.-DBs with MD in metals by Hyzhnyakov group have 0.5-5 eV

2.-The maximum energy transfer from Ar to Ge is 3.6 eV

3.- The activation energy for annealing an E center is about 1.36 eV

4.- The energy to anneal a defect has to remain localized up to 10^4 lattice units

5- The energy delivered by Ar atoms has to remain localized while traveling 10^4 lattice units

6.- Increasing the energy of the plasma does not enhance the effect, this is because DBs typically have a definite range or energies.

7.- At least stationary DB have obtained for Si and Ge with MD.

Some numbers

1.-Ion current can be measured, $\Phi_{Ar} = 1.25 \cdot 10^{13}\mathrm{cm}^{-2}\mathrm{s}^{-1} \approx 0.04 a^{-2} s^{-1}$

2.- DB creation efficiency: $\gamma :\quad \Phi_{DB} = \gamma \cdot \Phi_{Ar} \quad ; \quad \gamma < 1$

3.-Number of breathers: $n_{DB} = \dfrac{\Phi_{DB}}{c_s} \approx \gamma 2.3 \cdot 10^{7}\,\mathrm{cm}^{-3}$

$$4. - \text{Phonons}: \quad E_{ph} = 0.035\mathrm{eV} \quad \mathrm{n_{ph}} = \frac{3n_{Ge}}{\exp(E_{ph}/k_B T) - 1} \approx 4.6 \cdot 10^{22}\mathrm{cm}^{-3}$$

$$\text{For}\,\gamma = 1 \qquad -\frac{1}{N_T}\frac{dN_{T,DB}}{dt} \approx 2 \cdot 10^{-4} s^{-1} \qquad -\frac{1}{N_T}\frac{dN_{T,RT}}{dt} \approx 2 \cdot 10^{-11} s^{-1}$$

Relative annealing efficiency per DB or phonon: ~10^{22}

Relative annealing efficiency per eV of DB or phonons: ~10^{20}

Interaction cross-section and energy delivered by a breather

Interaction cross-section σ

$$-\frac{dN_T}{dt} = \sigma N_T \Phi_{DB} \exp\left(-\frac{E_0 - \Delta}{k_B T}\right)$$

Interaction cross-section $\sigma = \alpha\sigma_0 \quad ; \quad \alpha > 1$

Minimal interacion cross-section $\sigma_0 = n_{Ge}^{-2/3} \approx 10^{-15}\,\mathrm{cm}^2$

Apparent diminution of the activation energy because of DB interaction: Δ

$$-\frac{dN_T}{dt} = \alpha\gamma\sigma_0 N_T \Phi_{ions} \exp\left(-\frac{E_0 - \Delta}{k_B T}\right) \qquad \alpha, \gamma, \Delta \quad \text{unknown}$$

$$-\frac{dN_T}{dt} = \sigma_{ions} N_T \Phi_{ions} \qquad \sigma_{ions} \approx \frac{1}{50}\sigma_0 \approx 1.5 \cdot 10^{-17}\,\mathrm{cm}^2$$

For $\alpha\gamma = 1, \quad \Delta \approx 1.2\,\mathrm{eV}$

Conclusions:

0.- Plasma of 4eV produces annealing of defects very deep in Ge

Likely conclusions:

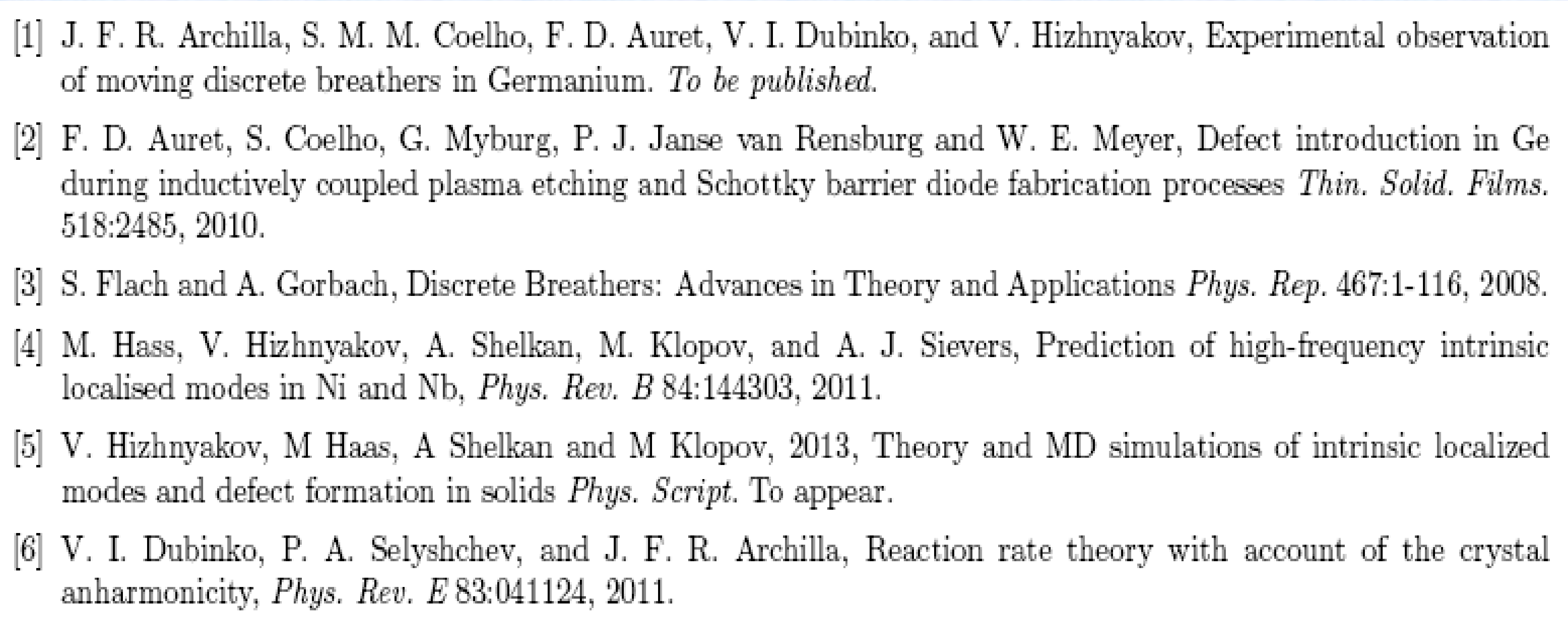
1.- 4 eV Ar hits produce DB in Ge with very high efficiency

2.- DB of energy ~3eV travel distances of the order of at least 10^4 lattice units

3.- The annealing efficiency of DB with respect to phonons is extremely large

4.- The energy delivered by a DB to a defect is ~1.2 eV

References



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