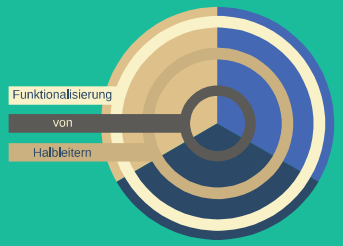

DFG

Philipps Universität Marburg

Peculiarities of the photoluminescence line shape in Ga(N,As,P)/GaP: Experiment and Monte Carlo simulations

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GRK Seminar, Kunze-Hof, Stadland, 2017

Monte Carlo studies

Computer simulations of disordered materials properties:

- Charge Transport properties
- Optical properties

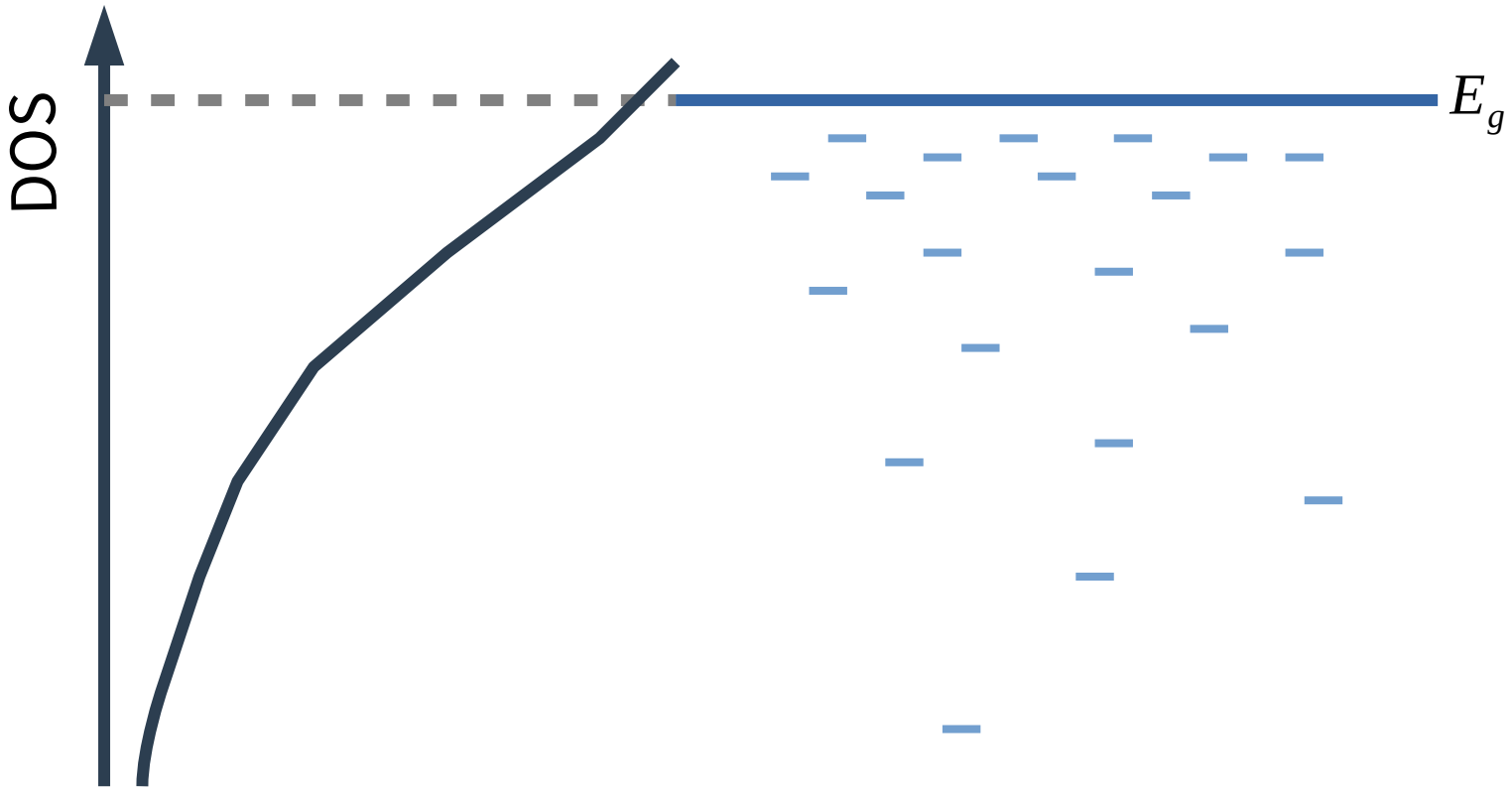
Ga(N,As,P)/GaP PL

Outline

- Intro
- Baranovskii – Eichmann – Thomas(BET) model
- Modified BET – model : Two scales of disorder
- Alternative approach : Complex DOS and T-dependent non-radiative recombination
- Conclusions

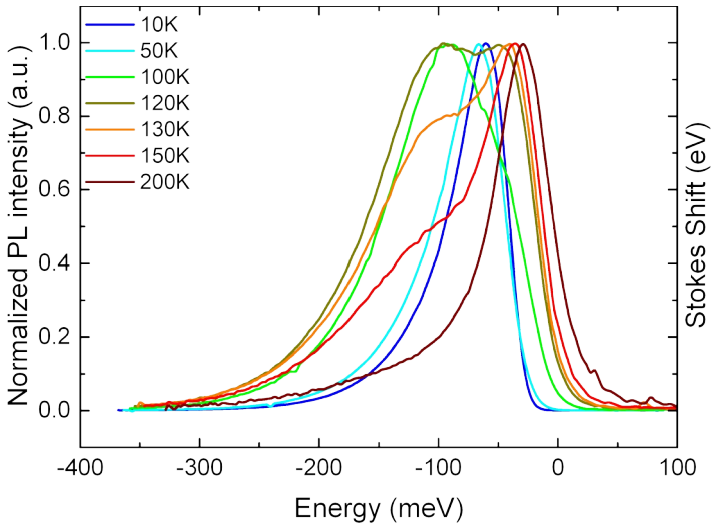
Disorder-induced localized states

Tale of localized states (LS) due to disorder:

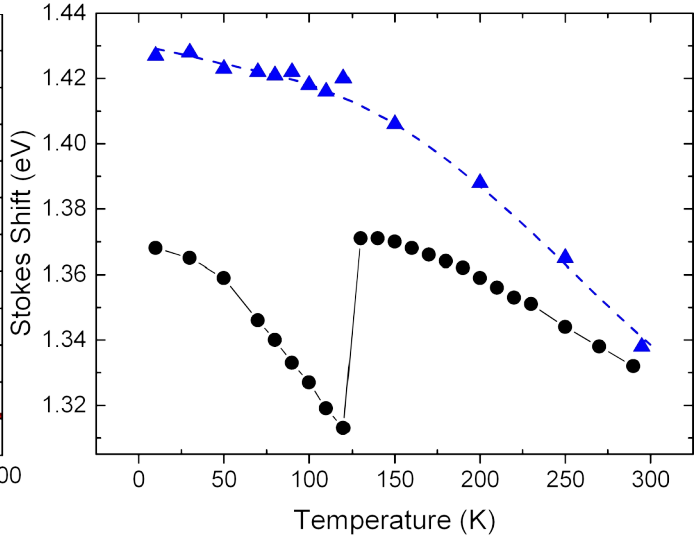


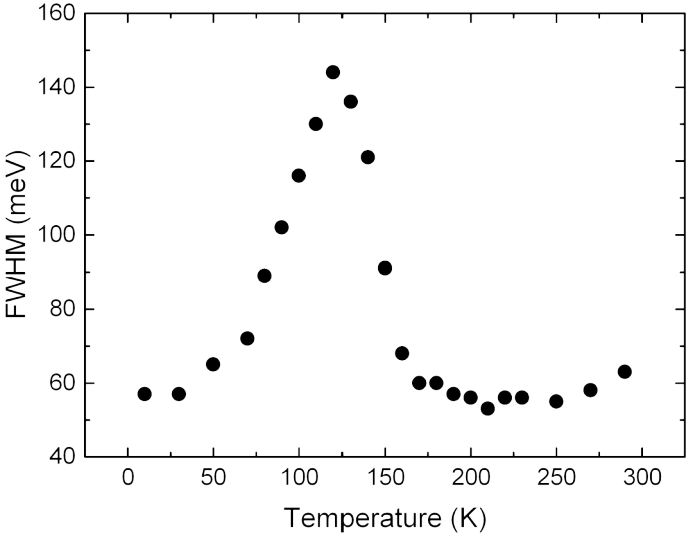
Experimental measurements

PL Spectra:



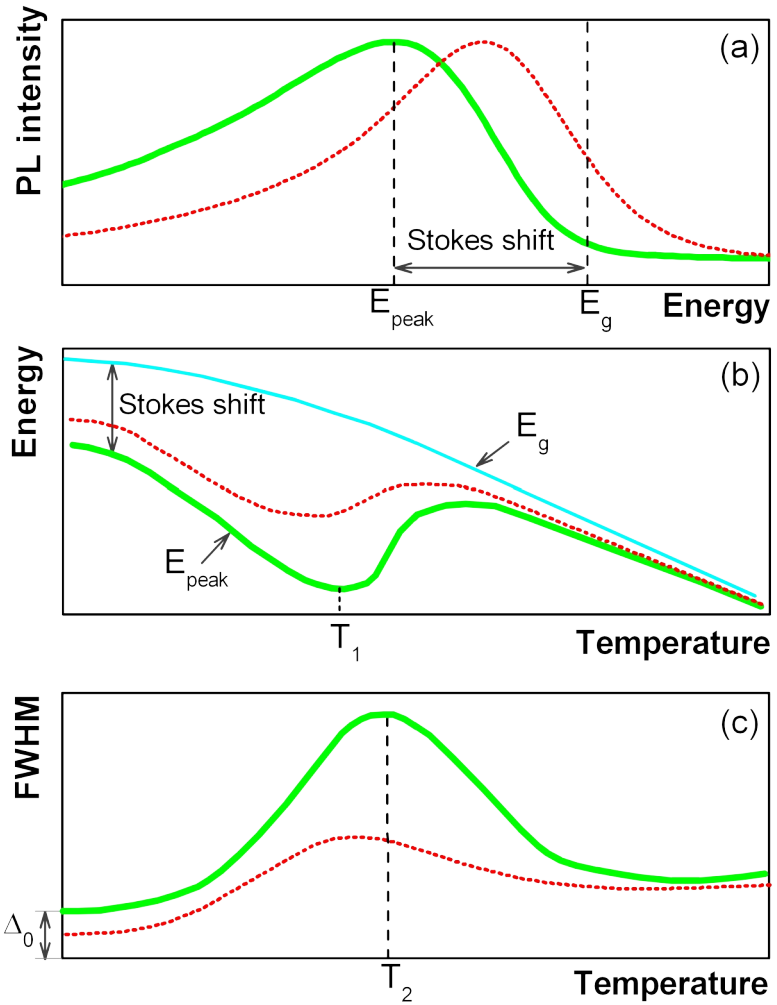
PL Features:





Karcher C, Jandieri K, Kunert B, Fritz R, Zimprich M,Volz K, Stolz W, Gebhard F, Baranovskii S D and Heimbrodt W 2010 Phys. Rev. B ***82*** *245309*

Peculiarities of PL in disordered material



(a) Schematic shapes of the PL spectra;

(b) temperature-dependent PL peak position;

(c) PL linewidth;

Green solid line – low excitation
Red doted line – high excitation

BET - model

Assumptions:

- Traps distributed randomly in energy and coordinates;
- No correlations between energy and spatial positions of traps are assumed;
- Electrons and holes are coupled in form of excitons.

Dimensionless parameters: $\frac{E_0}{kT}$ Na^2 $\nu_0\tau_0$

Processes:

- Capture to localized states (LS);
- Activation to extended states;

$$\nu_i = \nu_0 \exp\left(\frac{E_i}{kT}\right)$$

- Hopping transitions between LS;

$$\nu_{ij} = \nu_0 \exp\left(\frac{-2R_{ij}}{a} - \frac{E_j - E_i + |E_j - E_i|}{2kT}\right)$$

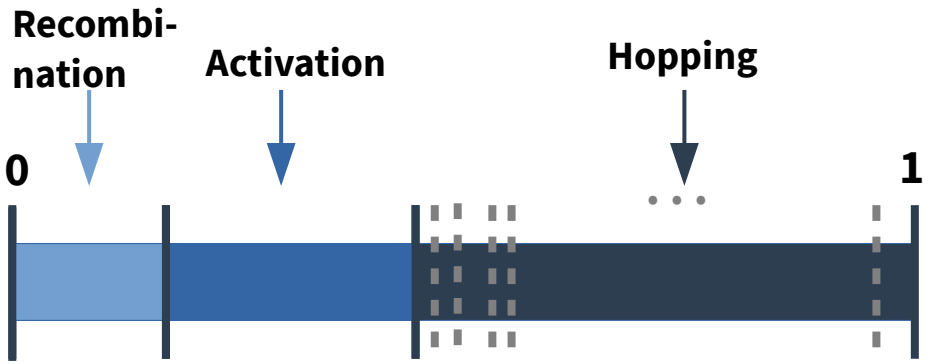
- Recombination;

*Baranovskii S D, Eichmann R and Thomas P 1998 Phys.Rev. B **58**13081*

BET - model

KMC Simulation algorithm:

- *Step 1:* Generate LS's ;
- *Step 2:* Set particle to random site;
- *Step 3:* Throw random number to select next event;
- *Step 4:* Throw random number to generate event's time;
- Repeat *Steps 3-4* until recombination.



$$\Delta t_i = -\ln(x)\nu_i^{-1}$$

BET - model

Successfully applied to:

- **Quantum wells:**

  GaInNAs/GaNAs, InGaN/GaN

- **Quantum dost:**

  InAs/GaAs

- **Bulk materials:**

  GaP(N)

Key feature:

Relations between energy scale of disorder(E) and temperature maximums (T1 and T2)of PL Stokes Shift / FWHM.

Feature	Relation to E/k
T1 (Stokes Shift max)	~ (0.7 – 0.8)
T2 (FWHM max)	~ (1.1 – 1.2)
FWHM (at low T)	~ 2.5

Rubel O, Galluppi M, Baranovskii S D, Volz K, Geelhaar, L, Riechert H, Thomas P and Stolz W 2005 J. Appl. Phys. ***98*** *063518*

Dawson P, Rubel O, Baranovskii S D, Pierz K, Thomas P and Goebel E O 2005 Phys. Rev. B ***72*** *235301*

Dawson P, Goebel E O, Pierz K, Rubel O, Baranovskii S D and Thomas P 2007 Phys. Stat. Sol. b 244 2803

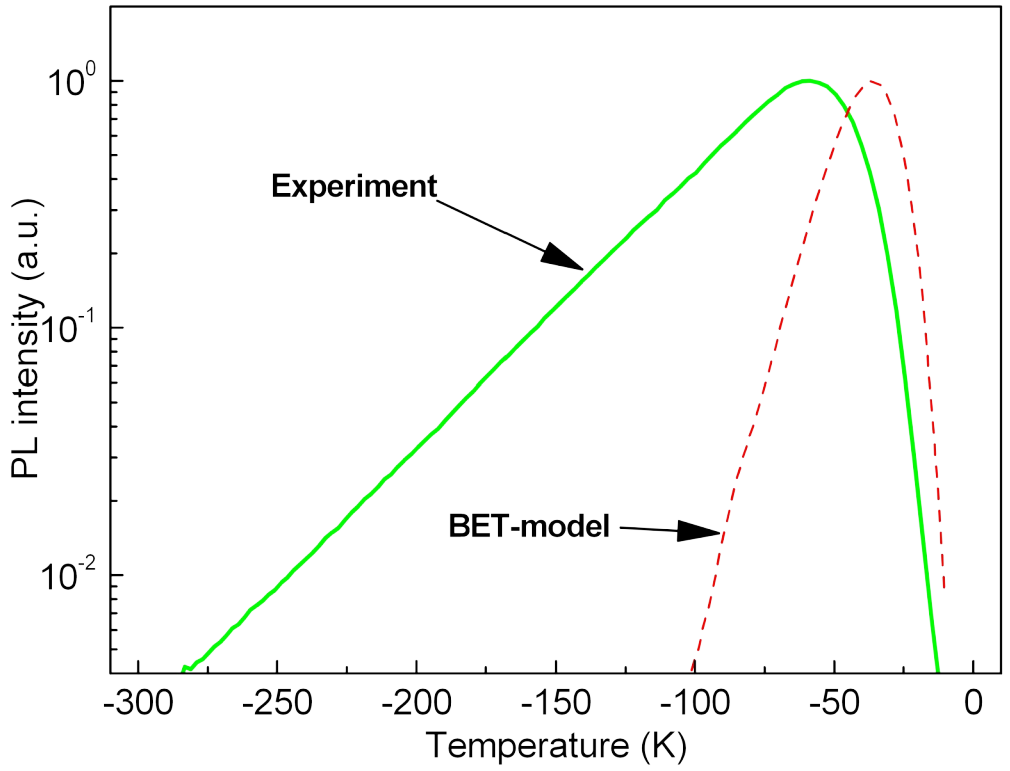
Problems of BET – model for Ga(N,As,P)

Problem:

Relations between PL features and energy parameter of disorder doesn't work!

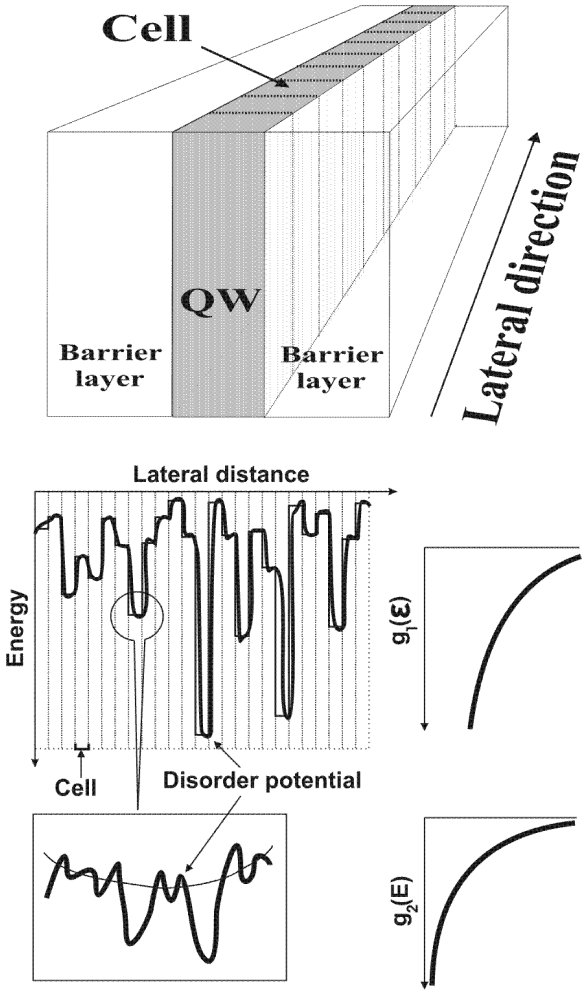
Relation between E_0 and PL features	PL feature (meV)	E_0 (meV)
$k_B T_1 = (0.75-0.80) E_0$	10.4	13
$k_B T_2 = (1.10-1.15) E_0$	10.4	9
$\mathrm{FWHM}(0) = (2.5-2.7) E_0$	57	22
$\beta = E_0^{-1}$	0.025[a]	40

[a]The value of β is given in $(\mathrm{meV})^{-1}$.



Karcher C, Jandieri K, Kunert B, Fritz R, Zimprich M,Volz K, Stolz W, Gebhard F, Baranovskii S D and Heimbrodt W 2010 Phys. Rev. B ***82*** *245309*

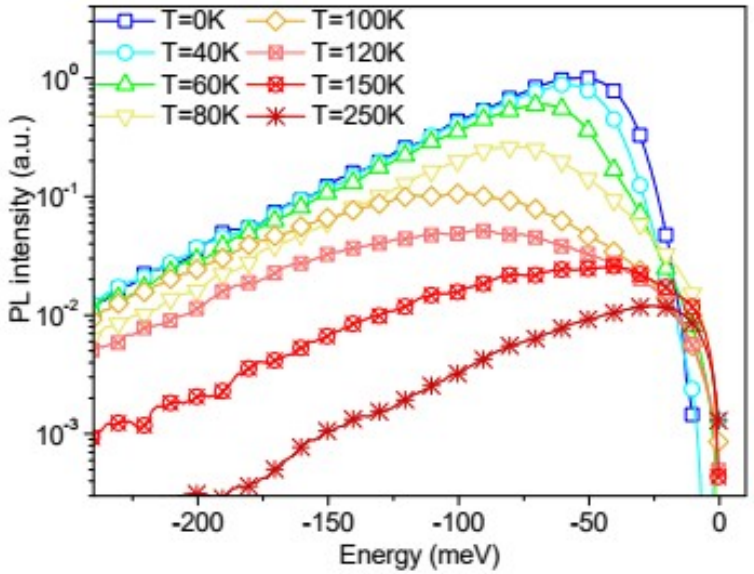
Modified BET – model: Two scales of disorder



DOS for double-scale of disorder:

$$G(E)=\frac{N_0}{\varepsilon_0-E_0}\left[\exp\left(\frac{E}{\varepsilon_0}\right)-\exp\left(\frac{E}{E_0}\right)\right]$$

Simulated spectrum:



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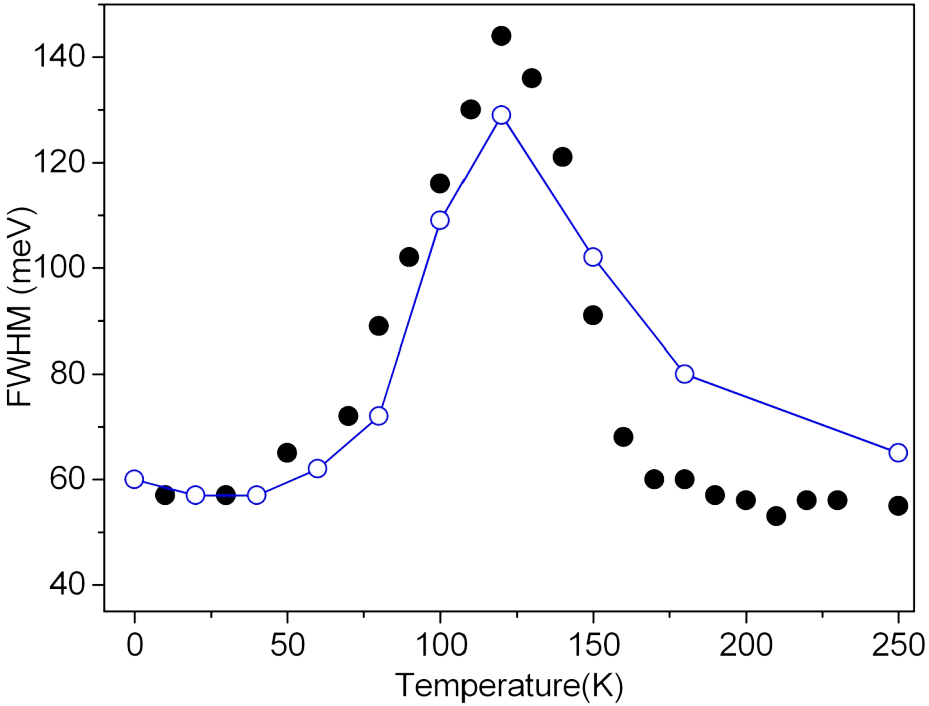
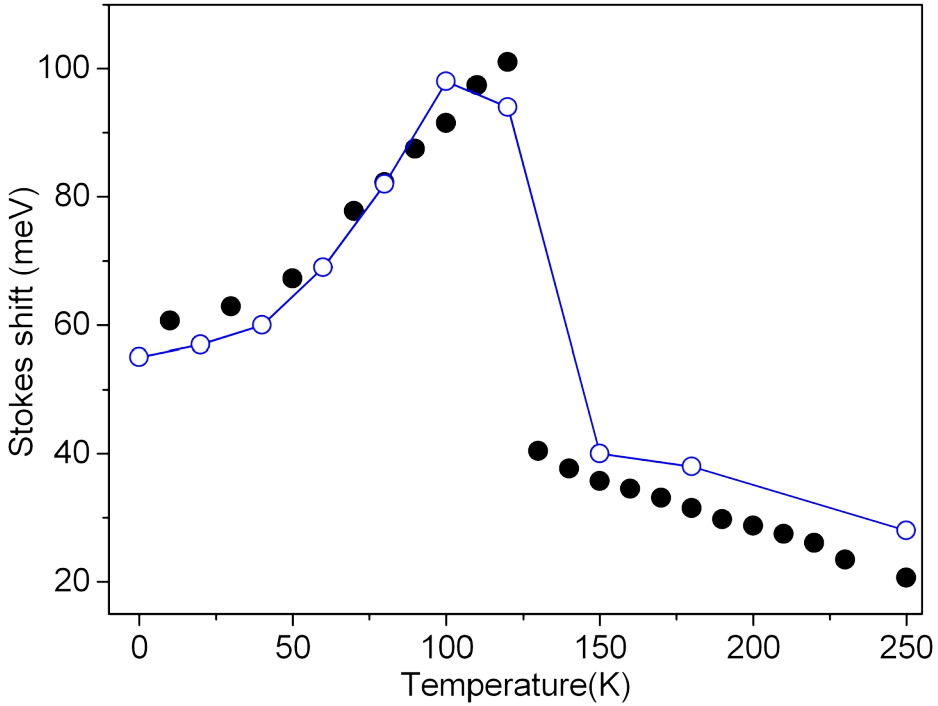
Modified BET – model. Two scales of disorder

Experimental results and simulation:

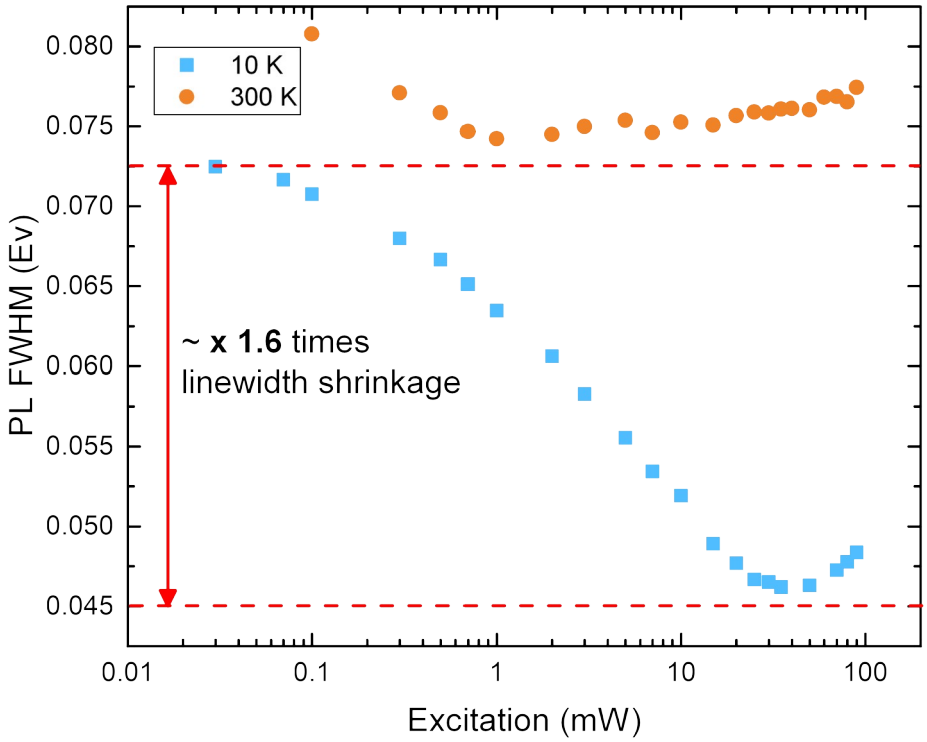




Karcher C, Jandieri K, Kunert B, Fritz R, Zimprich M,Volz K, Stolz W, Gebhard F, Baranovskii S D and Heimbrodt W 2010 Phys. Rev. B ***82*** *245309*

Ga(N,As,P) PL FWHM vs pump

Experimental result: At low temperatures *FWHM strongly decreases* along with the increase of the Peak Energy, when increasing the excitation power



Similar behavior reported for GaAsBi/GaAS:

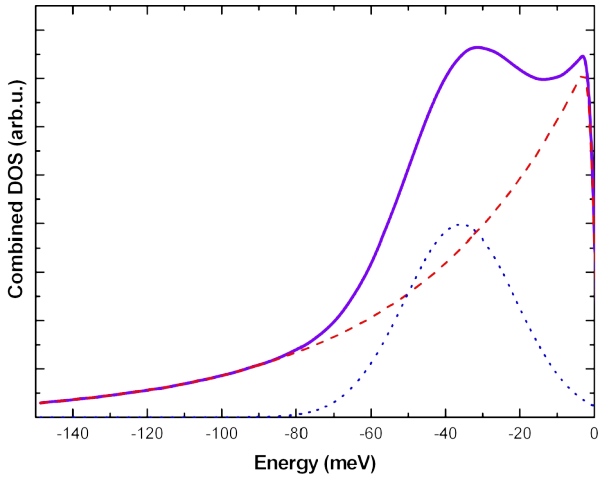
Mazur Y I *et al* 2013 *J. Phys. D: Appl. Phys.* **46** 065306

Modified BET – model: Complex DOS

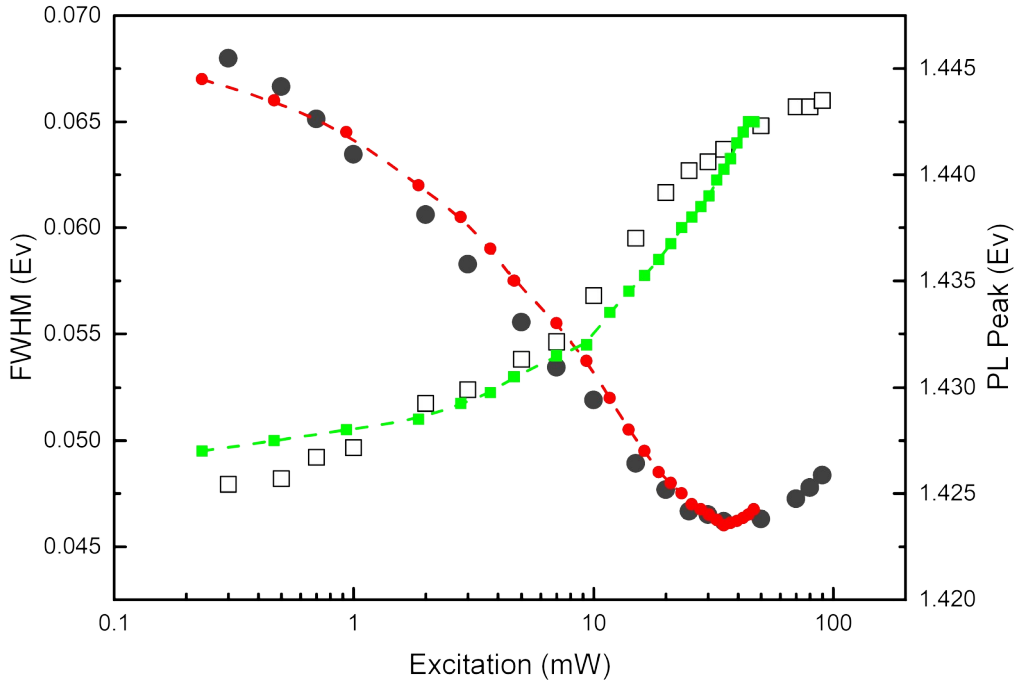
Complex DOS:

Parameter	Value	Description
N_0/N_1	7/3	Fitting parameter
E_0	46 (mEv)	Experimentally determined
E_1	36 (mEv)	Fitting parameter
σ_1	15 (mEv)	Fitting parameter
$N\alpha^2$	0.06	Fitting parameter
$\nu_0\tau_0$	$3.5 \cdot 10^3$	Experimentally determined

$$g(E) = A_0 \exp\left(\frac{E}{E_0}\right) + A_1 \exp\left(\frac{(E_1 - E)^2}{2\sigma_1}\right)$$



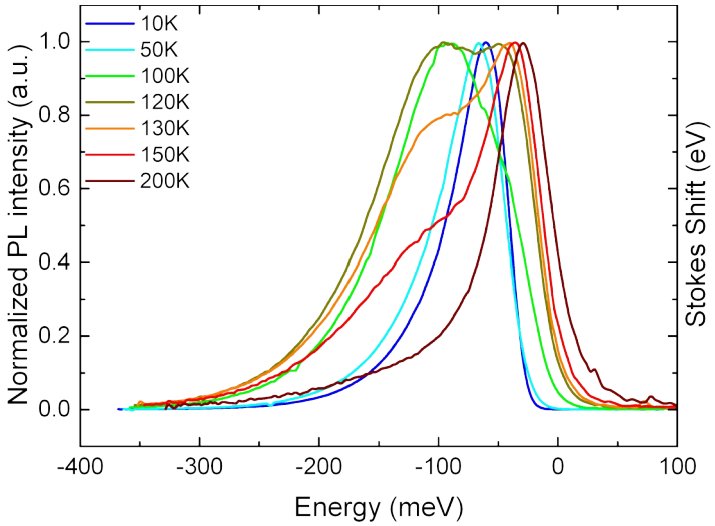
Simulation results:



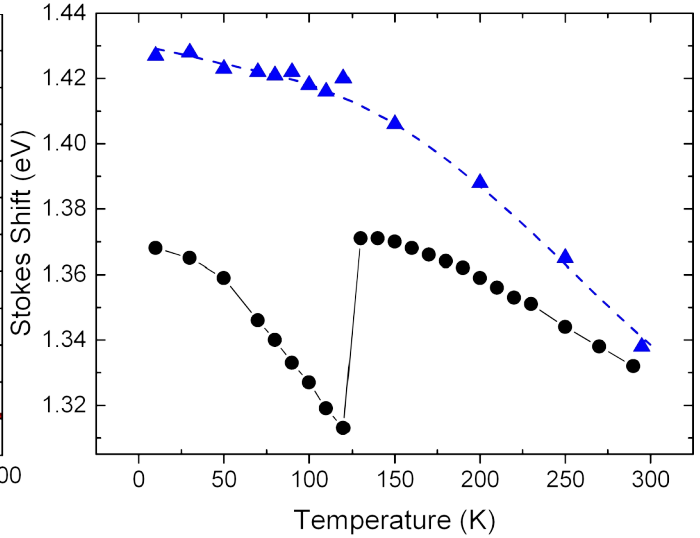
Valkovskii V V, Shakfa M K, Jandieri K, Ludewig P, Volz K, Stolz W, Koch M and Baranovskii S D , 2017 *J. Phys. D: Appl. Phys* **50** 025105

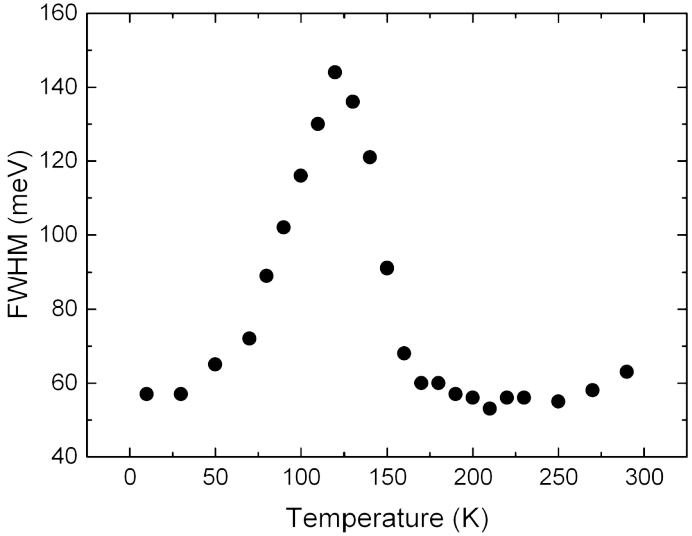
Experimental measurements

PL Spectra:



PL Features:





*Karcher C, Jandieri K, Kunert B, Fritz R, Zimprich M,Volz K, Stolz W, Gebhard F, Baranovskii S D and Heimbrodt W 2010 Phys. Rev. B **82** 245309*

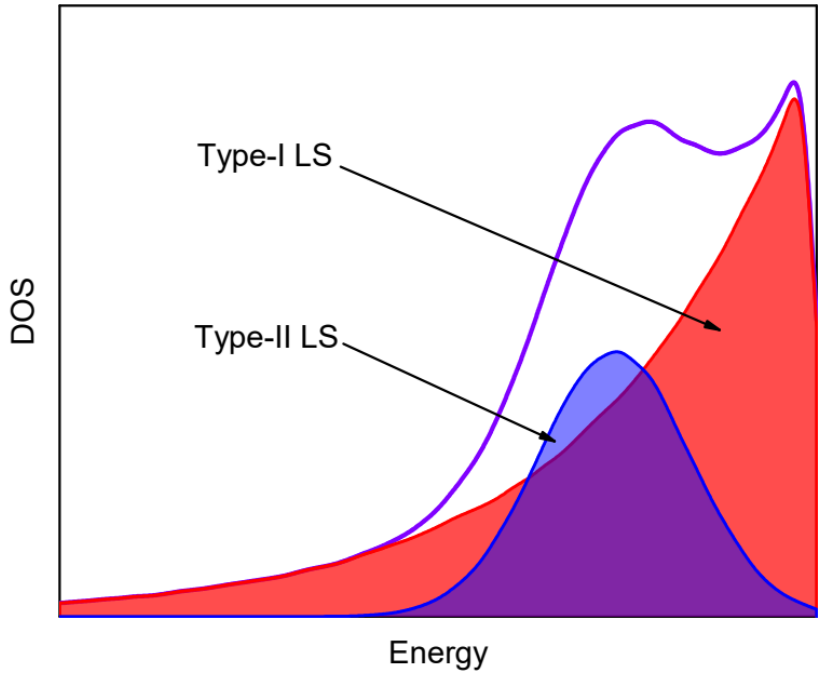
Modified BET – model. Two types of LS

Assumptions:

- Many particle system;
- Complex DOS given by:

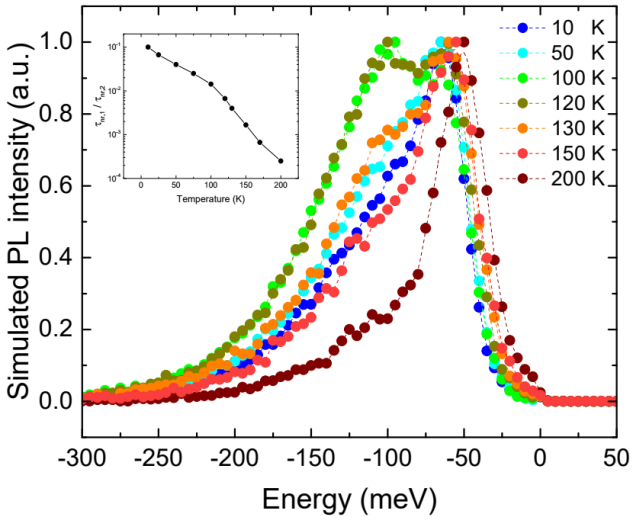
$$g(E)=A_0\exp\left(\frac{E}{E_0}\right)+A_1\exp\left(\frac{(E_1-E)^2}{2\sigma_1}\right)$$;

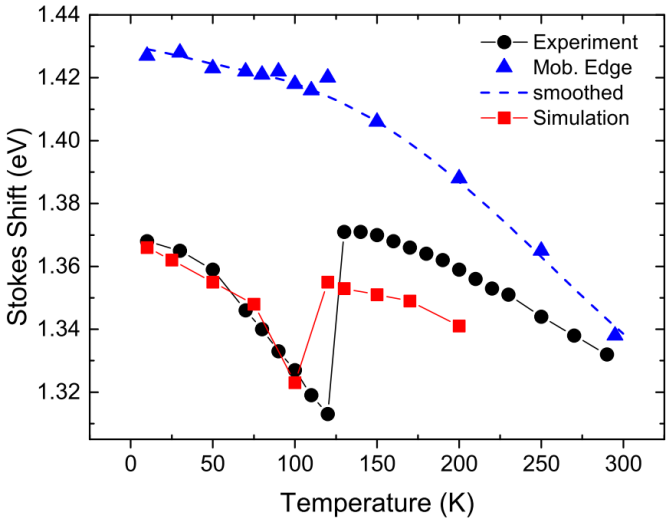
- Two types of the LS;
- Strong temperature dependence of non-radiative recombination;
- New parameter – ratio of non-radiative recombination rates $\tau_{nr,1}/\tau_{nr,1}$.

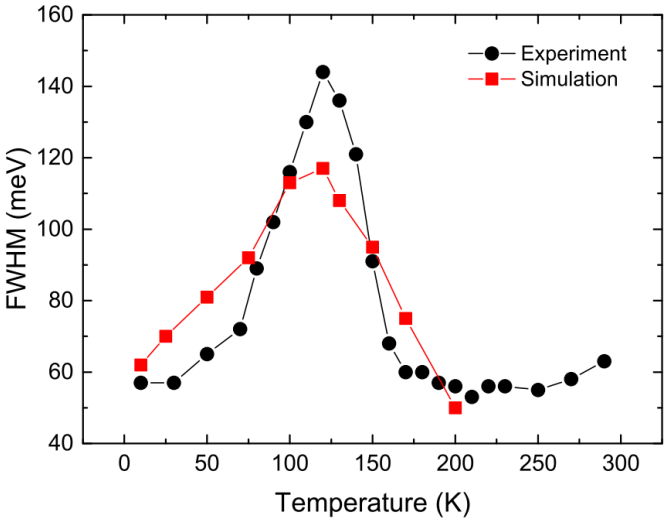


Modified BET – model. Two types of LS

Simulation results :







Parameter	Value
N_0/N_1	6/4
E_0	40 [meV]
E_1	38 [meV]
σ_1	16 [meV]
$N\alpha^2$	0.25
$\nu_0\tau_r$	10^3

Conclusions

- We have studied PL features of Ga(N,As,P) quantum wells using Kinetic Monte Carlo method;
- Principal problems of the original BET – model has been revealed;
- The original model has been refined, assuming the following:
  - ***Two types of LS with non-monotonous (exponential-plus-Gaussian) DOS;***
  - ***Strongly different temperature dependencies of non-radiative recombination rates at LS type-I and LS type-II***