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

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Motivation

Strongly non-monotonous behavior of the photoluminescence (PL) peak energy and photoluminescence full width at half maximum (FWHM) has been observed experimentally in Ga(N, As, P) multiple quantum well (QW) structures. At sufficiently low temperatures the PL FWHM strongly decreases along with the increase of the PL Peak Energy, when increasing the excitation power. Similar results were recently reported for InGaN/GaN [1] and GaAsBi/GaAs[2].

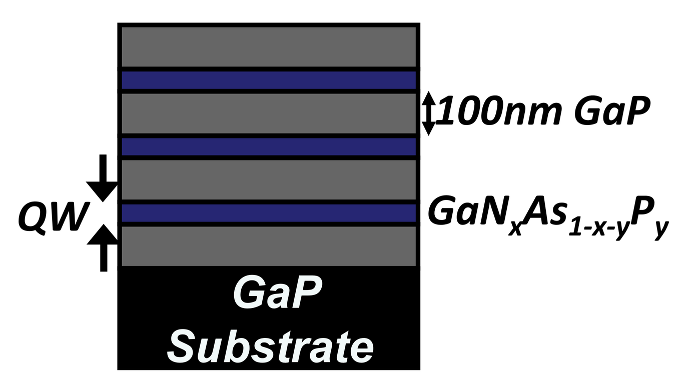
Another feature, which requires explanation, is presence of two peaks in PL spectra. When temperature is increased PL peak shifts from one to another. Such a behavior leads to sharp leap in PL Stokes Shift dependence on temperature.

To reveal the provenance of such a PL behaviour the Kinetic Monte Carlo (KMC) method is applied to directly simulate the processes of exciton hopping relaxation and recombination in the disorder-induced tail of localized states (LS).

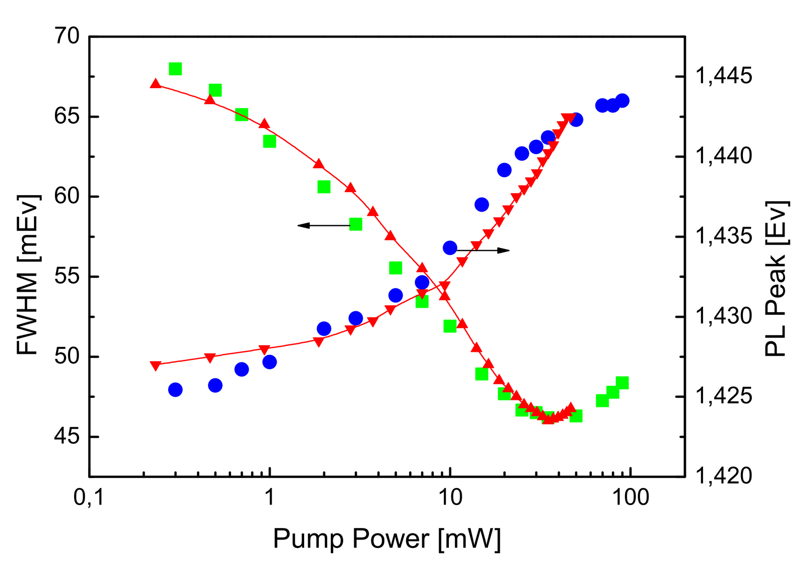
Experiment and Simulation

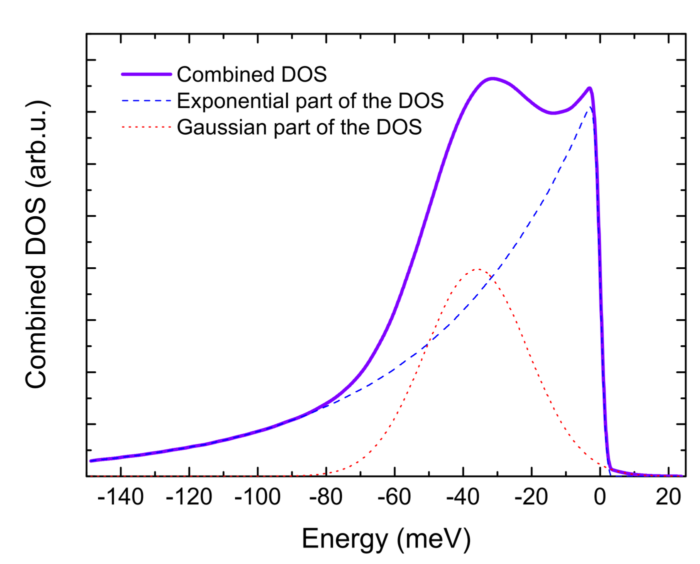
Specimens under study:

Ga(N, As, P)/GaP multiple QW, grown on (001)-oriented GaP substrate by MOVPE method.

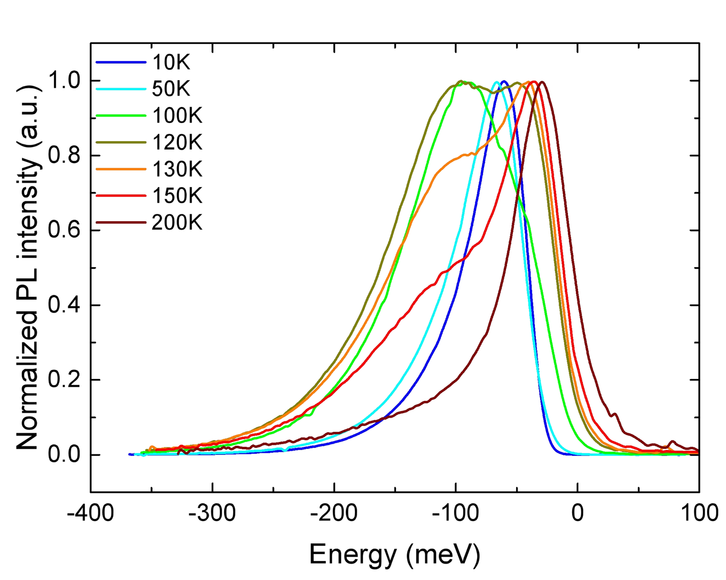


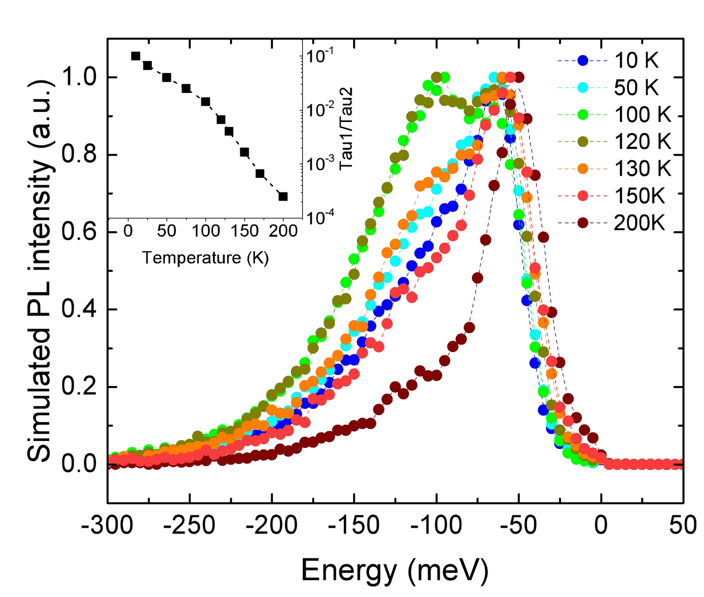
Measurments and Simulations:



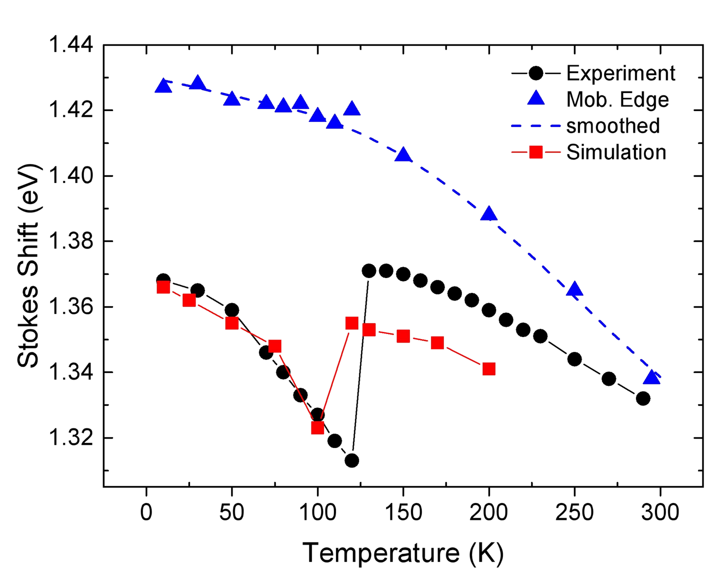


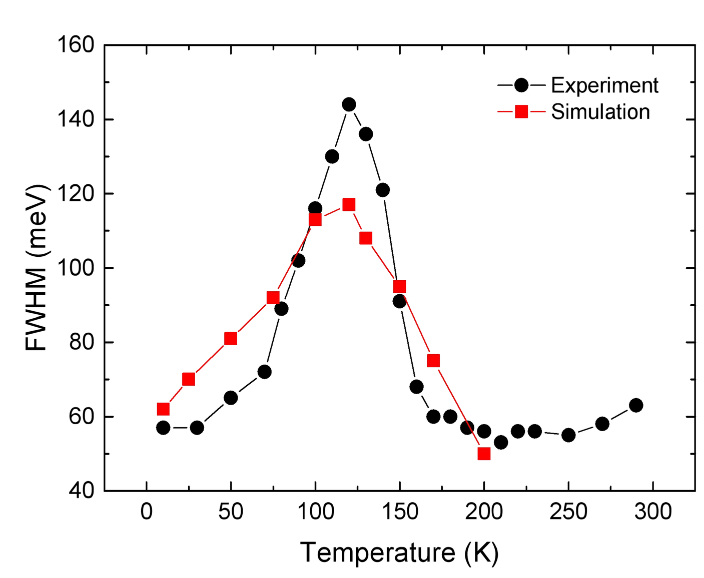
Excitation dependencies(left fig.) of the PL FWHM(green rectangles) and the PL peak(blue circles) along with KMC simulations; Shape of the DOS in KMC (right fig.)





Pl-spectrum at temperature range: 10 - 200 K
Experiment(left) and KMC simulation(right);





Temperature depdendences of Stokes Shift(left) and FWHM(right) along with KMC simulation.

Theoretical model:

Modified Baranovskii-Eichmann (BE) model of the exciton hopping relaxation through the localized states (LS) [3] is employed to explain experimentally observed results.

The key inputs of the conventional BE-model are the following:

- The trapping sites are randomly distributed in space;
- No correlations between energies of sites and their spatial positions;
- The density of states (DOS) given by $g(E) = A_0 f_0(E, E_0)$;
- Electron-hole pairs are strongly correlated in the form of excitons;
- PL lineshape is determined by hopping transitions and recombination;
- Single-particle system;

Modification of the BE model:

- Many-particle system;
- The Composite Two-component Density of States (DOS) instead of the Single Component DOS;

$$g(E) = A_0 f_0(E, E_0) + A_1 f_1(E, p_1, p_2 \dots) \qquad (1)$$

A_i - *normalization factors;*

$E_0, p_1, p_2, \dots$ - *disorder parameters*

- Two types of LS;
- Temperature dependent non-radiative recombination rates.

Simulation algorithm details:

KMC Simulation, based on the algorithm given in *Ref. [3]*, including modifications to describe many-particles system.

Considered processes:

•Exciton activation to the extended states;

•Exciton localization;

•Exciton hopping transition between localized states;

•Exciton recombination.

Parameters of the model:

$N\alpha^2, \nu_0\tau_0, N_0/N_1, E_0, p_1, p_2 \dots$

N – concentration of LS;

α – localization length (order of Bohr radius);

ν_0 – attempt to escape frequency;

τ_0 – typical exciton lifetime;

N_i – part of LS with distribution f_i;

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

Conclusions and References

•The combined exponential-plus-gaussian DOS has been revealed as necessary to provide a good agreement between experiment and theory;

•Such a shape of the DOS can be interpreted as the indication of two types of LS;

•In order to explain temperature dependence of PL peculiarities, temperature dependent non-radiative recombination rates for two types of LS has been introduced to modify standart BE model.

References:

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Supported by German Research Foundaion (DFG)
GRK - 1782