

# Abstract

## Calculations of electronic band-structure and optical gain for an active region of modern semiconductor lasers

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In this dissertation, electronic band-structures and material optical gain spectra are calculated for semiconductor structures, especially quantum wells based on GeSn/Ge and BGaAs/GaP material systems, which can be integrated with a Si substrate. The work is focused on the analysis of the structures for applications as active regions of Si-integrated lasers.

The work contains: a presentation of applied models and schemes together with analysis of their influence on the gain calculations, and discussion of the results obtained for chosen semiconductor structures together with presentation and discussion of used material parameters.

Calculations of electronic band-structures is performed based on multi-band  $k \cdot p$  models and envelope function approximation expressed in a basis of plane-waves. Strong influence of  $L$  and  $\Delta$  valleys on quasi-Fermi levels is taken into account via chosen algorithm of solving Schrödinger and Poisson equations self-consistently. Optical gain spectra are calculated based on Fermi's golden rule with detailed consideration of the electronic bands shapes and selection rules for each optical transition. Reliability of chosen models is justified through the analysis of their influence on the calculated optical gain.

The results of this work are: tested method of calculation of material-optical-gain spectra for semiconductor structures with significant role of  $L$  and  $\Delta$  valleys, set of material parameters describing constituent materials of analysed structures, and an analysis of electronic band-structures and optical gain spectra of chosen semiconductor structures.

The performed research confirmed that the structures, especially the quantum wells, based on GeSn/Ge or BGaAs/GaP are attractive structures for further experimental work, since it is shown that optical gain can be achieved in these structures with parameters of the system that are typically achievable.