University of Belgrade
Institute of Physics Belgrade
Kopaonik, March 13-16, 2022

Book of Abstracts

15th Photonics Workshop

(Conference)

PHOTONICS
CENTER

15th Photonics Workshop (2022)

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Kopaonik, Serbia, March 13-16, 2022

Publisher, 2022:

Institute of Physics Belgrade

Pregrevica 118

11080 Belgrade, Serbia

Editors:

Dragan Lukić, Marina Lekić, Zoran Grujić

ISBN 978-86-82441-55-7

Printed by:

NEW IMAGE d.o.o.

Tošin Bunar 185, Belgrade

Number of copies: 55

CIP - Каталогизација у публикацији - Народна библиотека Србије, Београд
535(048)
681.7(048)
66.017/.018(048)
PHOTONICS Workshop (15; 2022; Kopaonik)
Book of Abstracts / 15th Photonics Workshop, (Conference), Kopaonik,
March 13-16, 2022; [editors Dragan Lukić, Marina Lekić, Zoran Grujić]. -
Belgrade: Institute of Physics, 2022 (Belgrade: New image). - 72 str.:
ilustr.; 25 cm
Tiraž 55. - Registar.
ISBN 978-86-82441-55-7
a) Оптика - Апстракти b) Оптоелектроника - Апстракти c) Технички
материјали - Апстракти

COBISS.SR-ID 60055049

Numerical modeling of new oxide-based heterostructures for use in QCL devices

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Abstract. Semiconductor devices operating in the terahertz (THz) and near/mid infrared (IR) parts of the optical spectrum have been continuously explored and improved during the previous two decades [1-3]. Multiple new material platforms are being experimentally and theoretically investigated as candidates for room temperature operation of THz devices. One of the materials under recent consideration is ZnO due to its wide direct bandgap and high exciton binding energy. In this contribution we illustrate the use of a modified version of the Newton-Raphson method to numerically and self-consistently solve a system of Schrödinger-Poisson equations for a structure consisting of coupled ZnO–based quantum wells. The results obtained are compared with the experimental data available in the literature, after which the influence of layers' thickness and doping profile on the bound states energies is analyzed. Additionally, the impact of the external electric field applied to the structure is assessed in order to determine the doping profile and well/barrier thicknesses that would be most promising for quantum cascade laser applications. Finally, we evaluate the absorption due to intersubband transitions between the bound states.

Acknowledgments

The authors acknowledge support from Ministry of Education, Science and Technological Development (Republic of Serbia), "Multi-Scale Modeling of Terahertz Quantum Cascade Laser Active Regions", Multilateral scientific and technological cooperation in the Danube region 2020-2021, and "DEMETRA: Development of high-performance mid-IR / THz quantum cascade lasers for advanced applications", Science Fund of the Republic of Serbia, Serbian Science and Diaspora Collaboration Programme: Knowledge Exchange Vouchers.

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