Tuning the crystal structure, optical band gap and persistent luminescence performance of Cr^{3+}-doped $LiGa_5O_8$ spinel by adding aluminum and indium

A. Karabut[1], H. Zhydachevska[1], Ł. Wachnicki[1], V. Hreb[2], L. Vasylechko[2],
Yu. Hizhnyi[3,4], T. Shevtsova[3], Ya. Zhydachevskyy[1,#]

[1] Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
[2] Lviv Polytechnic National University, Lviv, Ukraine
[3] Donetsk Institute for Physics and Engineering of NAS of Ukraine, Kyiv, Ukraine
[4] Taras Shevchenko National University of Kyiv, Kyiv, Ukraine

The possibility of tuning the optical band gap, crystal structure and persistent luminescence performance of Cr^{3+}-doped $LiGa_5O_8$ spinel by partially replacing Ga with Al and/or In has been studied extensively. For this purpose, a series of Cr^{3+}-doped $Li(Ga_{1-x-y}Al_xIn_y)_5O_8$ ($x = 0…0.5$; $y = 0…0.1$) microcrystalline phosphors were synthesized using a conventional solid-state reaction method and characterized by powder X-ray diffraction and luminescence techniques. The DFT-based electronic structure calculations were carried out for the same $Li(Ga_{1-x-y}Al_xIn_y)_5O_8$ compositions, and the results were compared with the experimental ones. Based on the studies performed, the mechanism of Al and In incorporation into the $LiGa_5O_8$ spinel structure, as well as the tuning of the crystal lattice parameters, local structure of M^{3+} (M = Ga, Al, In) cations and optical band gap of the material have been established. The multicenter structure and the broadening of the local structural disorder of the octahedrally coordinated Cr^{3+} centers observed in this case have been confirmed by the high-resolution, low-temperature photoluminescence measurements. Band gap engineering through alterations in the chemical composition of the $LiGa_5O_8$ spinel, as well as the depth of the native point defects responsible for charge trapping, allows for the efficient tuning of the thermoluminescent and persistent luminescent properties of $Li(Ga_{1-x-y}Al_xIn_y)_5O_8:Cr^{3+}$ phosphors. Thus, the room-temperature persistent luminescence performance of the phosphors modified by the addition of Al and annealing in an oxygen-free atmosphere was increased threefold compared to the pristine $LiGa_5O_8:Cr^{3+}$ phosphor synthesized under the same conditions.

The work was supported by the Polish National Science Centre (project no. 2024/53/B/ST11/01108), the Ministry of Education and Science of Ukraine (project DB/GALIO no. 0125U001768), and the European Research Executive Agency (HORIZON-MSCA-2023-SE-01 Project no. 101182995). The authors gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Centre: ACK Cyfronet AGH) for providing computer facilities and support within the computational grant no. PLG/2024/017683.

corresponding author: zhydach@ifpan.edu.pl