

Role of Defects in Formation of the Luminescence Properties of Zinc Molybdate Crystals

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The luminescence properties of zinc molybdate crystals ZnMoO_4 are intensively studied at present since these crystals are considered as perspective scintillation materials for various experiments in particle physics. The luminescence spectra of undoped ZnMoO_4 crystals usually reveal two components peaking near 530 and 620 nm. According to current opinion, the short-wavelength component originates from radiation annihilation of self-trapped excitons localized on MoO_4 groups of the crystal. However, the origin of the long-wavelength component is still the subject of discussion. According assumption made by several authors, this component should be related to existence the oxygen vacancies in the crystal lattice which form the oxygen-deficient molybdate groups MoO_3 . The present work is aimed to examine this assumption in complex experimental and computational studies. Dependences of intensity of the long-wavelength emission component and other luminescence characteristics of zinc molybdate on concentration of the oxygen vacancies are analyzed as result of luminescence spectroscopy studies carried out for the set of samples synthesized at different conditions.

The polycrystalline samples of ZnMoO_4 with varying concentration of structural defects were synthesized by solid-state reaction method. The luminescence properties were studied in the VUV region of excitation photon energies on SUPERLUMI station at HASYLAB (Hamburg, Germany). Additional bands in the optical absorption spectra were characterized by diffuse reflectance spectroscopy. The influence of several kinds of defects (V_o , V_o+V_{Zn} and W_{Mo}) on the electronic structure of ZnMoO_4 crystal was studied by FP-LAPW method [1].

As the experimental results show, the increase of the oxygen vacancies concentration leads to increase of the relative intensity of the 620 nm emission component of ZnMoO_4 and to appearance of additional bands in luminescence excitation spectra in 3.7 – 4.7 eV range of exciting photons energies. The electronic structure results indicate existence of the electronic states of oxygen-deficient MoO_3 groups in the crystal band-gap. Obtained results and their analysis support assumption on the oxygen vacancy-related origin of the long-wavelength emission component of zinc molybdate.

[1] P. Blaha et al, ISBN 3-9501031-1-2, 2001.