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YUCOMAT 2021

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X-ray properties spectroscopy and electron structure of $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ garnet with doped Ce (Eu)

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Crystals of $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ with the Ca-gallogermanate structure have a unique combination of physical properties - luminescent, laser, resilient, piezoelectric, and acoustic. Disordered trigonal compounds $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ activated with RE ions and transition elements are known as effective materials of quantum electronics, which combine the functions of generation and transformation of laser irradiation frequency. It stimulated the study of spectral - luminescent properties of transitional and RE metals impurity ions in these materials. However, the electronic structure, matrix luminescence of $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ crystals have not been sufficiently studied. The crystals were grown by Czochralski technique in the atmosphere of argon with adding oxygen using platinum crucible. The X-ray emission spectra of Ga (Ge) and Ce (Eu)L_{III}-edge in the $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ garnet with doped Ce 3 % and Eu 4% were obtained by a tube-spectrometer with X-ray coordinate detector of the original design. OK α -spectra in the $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ garnet were obtained by a SARF -spectrometer. Spectra of the core levels and the valence band in the $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ were measured by the "Kratos" X-ray photoelectron spectrometer. The X-ray spectral studies of the $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ have shown that the top of the valence band (near the Fermi level) is formed mainly by the outer electron *p*-states of Ga, Ge, and O, which intensity is sufficiently low. The middle of the valence band is formed by the *Ga 3d*-states with the *O2s*-states lying below them. These states are hybridized with the *4p*-states of Ga and Ge because of which they are *K β '*-satellite in *K β* - sub-band of *Ga* and *Ge*. The bottom of the valence band is formed by the *3d*-states of germanium, which contribution in chemical binding is insignificant. Alignment of the X-ray emission bands of Ga and Ge with photoelectron spectrum of valence electrons of the $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$ demonstrated satisfactory correspondence.