Excitation mechanisms of Mn-related luminescence in $YAlO_3$:Mn crystals

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The Mn-doped yttrium aluminum perovskite $YAlO_3$ has been intensively studied as a material for holographic recording, optical data storage and dosimetry of ionizing radiation with the use of thermally (TSL) or optically stimulated (OSL) luminescence [1, 2]. Manganese ions in $YAlO_3$:Mn crystals can be present in the form of Mn^{4+} ions in octahedral coordination (Al^{3+} sites) as well as Mn^{2+} ions in strongly distorted dodecahedral coordination (Y^{3+} sites). Despite a large volume of accumulated experimental data on optical and TSL properties, the excitation mechanisms and the energy transfer processes in $YAlO_3$:Mn crystals still require clarification as there were no direct results, neither theoretical nor experimental, regarding the positions of Mn energy states with respect to conduction or valence band of the $YAlO_3$ host.

The work presents experimental data measured in the VUV range of photoluminescence excitation (PLE), TSL creation, and optical absorption spectra of the $YAlO_3$:Mn crystals studied earlier in [2], as well as theoretical results on the electronic properties of a relevant set of Mn-relared point defects in $YAlO_3$ crystals. The geometry-optimized spin-polarized calculations of the electronic structures with use of DFT-based Plane-Wave Pseudopotential method and GGA-PBE exchange-correlation functionals were carried out in the super-cells approach. Various Mn-related point defects were modelled in the super-cells: single Mn_{Al} and Mn_Y substitutions, pair defect combinations of Mn_{Al} or Mn_Y with Hf_Y, Si_{Al}, Y_{Al} or V_O, as well as some triple-site defects like Mn_{Al}-Mn_Y-V_O, Mn_Y-V_O-Y_{Al} etc. Populations of Mn *d* defect levels in the particular defect complexes are analysed in order to understand the effect of charge trapping on the formation of Mn-related luminescence centers.

Results of the calculations are analysed together with the experimental data on PL, PLE, TSL creation, and optical absorption of $YAlO_3$:Mn crystals. On the basis of the made analyses the excitation mechanisms and the energy transfer processes involving Mn ions and intrinsic charge traps are discussed.

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