Combined crystal field and first principles studies of the Y_2O_2S phosphor doped with Yb^{3+} and Er^{3+}

G.A.Kumar[1], M.Pokhrel[1], C.-G.Ma[2], M.G.Brik[2], D.K.Sardar[1]

[1]Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, Texas 78249, USA
[2] Institute of Physics, University of Tartu, Tartu 51014, Estonia

Metal oxysulfides, such as Y_2O_2S, doped with the trivalent rare earth ions are attractive candidates for many photonics applications(1,2) and possesses several excellent optical properties along with better chemical stability, low toxicity and can be easily mass produced at low cost. For example Y_2O_2S:Yb, Er and Y2O2S:Eu are two of the best mass produced commercial up and down conversion phosphors widely used in the phosphor industry.

In the present work we report on the combined results of the experimental and theoretical studies of the Y_2O_2S phosphor doped with Yb^{3+} and Er^{3+} ions. The absorption and emission spectra were measured at low and room temperatures in the 300–1700 nm range. The energy levels of Er^{3+} were calculated using the crystal field theory; determined crystal field parameters allowed for getting good agreement with the experimental data (Fig. 1).

As an example of the performed analysis, we show in Fig. 1 the experimental absorption and emission spectra of $LaAlO_3$:Mn^{4+} together with the calculated Mn^{4+} energy levels (3). Good agreement between the calculated results and experimental spectra can be seen easily.

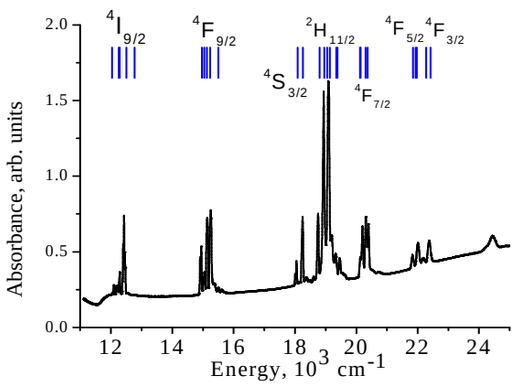

Fig. 1. Comparison of the 8 K experimental absorption spectrum of Y_2O_2S (solid line) with the calculated energy levels (vertical lines) of Er^{3+}.

Further treatment of the Er^{3+} optical properties in Y_2O_2S was performed using the Judd-Ofelt theory. The radiative life times and branching ratios were all determined and tabulated. In addition, the upconversion properties of the Y_2O_2S:Er, Yb system (which involve excitation of the Yb-Yb pair by infrared photons with a subsequent energy transfer to Er ions and emission of a visible photon) were also studied and the upconversion efficiency was measured experimentally using integrating sphere technique.

The first principles analysis of the Y_2O_2S phosphor was performed using the CASTEP module of Materials Studio. The structural, electronic, and optical properties were all calculated and compared with available experimental data. Thus, Fig. 2 shows the calculated band structure of Y_2O_2S with the indirect band gap of about 4.6 eV.

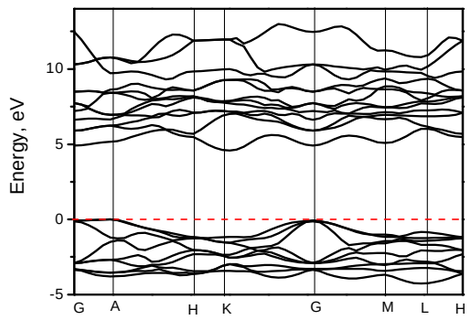

Fig. 2. The calculated band structure of Y_2O_2S. The indirect band gap is 4.6 eV.

The quality of the performed first principles analysis can be assessed by calculating the optical properties of the considered material. Fig. 3 presents the calculated dielectric function ε of Y_2O_2S in comparison with the experimental results from Ref. (3). The basic features of the Re(ε) and Im(ε) are well reproduced in our calculations.

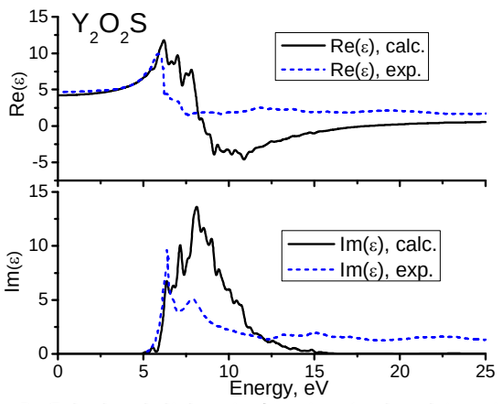

Fig. 3. Calculated dielectric function (real and imaginary parts) for Y_2O_2S (Experimental data are from Ref. (3).

We believe that such a combination of the semi-empirical crystal field theory with the first principles calculations can help in gaining a deeper insight into the electronic and optical properties of the Y_2O_2S:Er, Yb phosphor.

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