Reassignment of Ce^{3+} 5D Energy Levels

Peter A. Tanner[1], Lianshe Fu[1], Lixin Ning[2], Bing-Ming Cheng (鄭炳銘)[3], and Mikhail G. Brik[4]

[1]Department of Biology and Chemistry, City University of Hong Kong, Kowloon, China
[2]Dipartimento di Scienza dei Materiali, Universita di Milano-Bicocca, Cozzi, Italy
[3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan
[4]Fukui Institute for Fundamental Chemistry, Kyoto University, Takano, Japan

Ce^{3+}-doped YAG nanoparticles have been synthesized at relatively low temperatures by the co-precipitation and polymer-assisted sol-gel methods and characterized by FT-IR, XRD and XANES. Calcination of the product was carried out at temperatures between 800 °C to 1100 °C. Products calcined at the lower temperature contained a greater proportion of Ce^{4+} (as shown in Figure 1) and this contributed in part to the lower intensity of the characteristic yellow photoluminescence. The synchrotron radiation excitation spectrum of this yellow emission band exhibits bands due to Ce^{3+} absorption as well as the host band gap (Figure 2). The origin of a luminescence band at ca. 300 nm obtained under band-gap excitation has been rationalized. Previous assignments of the 5d electronic energies in YAG:Ce^{3+} have been critically assessed and in the light of new energy level and transition intensity calculations a revised assignment is put forward for the 5d energy levels (Figure 3).

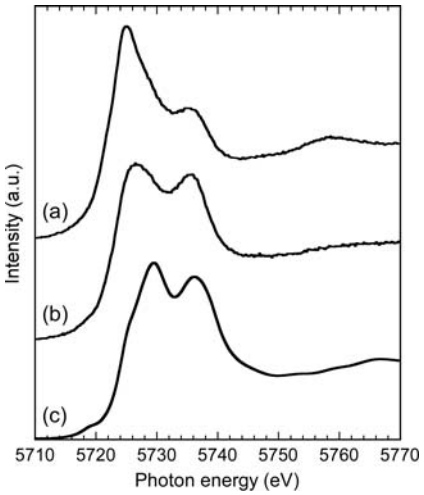

Figure 1. Ce-L_3 X-ray absorption near-edge structure in YAG: Ce^{3+} prepared by the polymer-assisted sol-gel method and calcined at (a) T = 1000 °C and (b) 800 °C in comparison to (c) CeO_2.

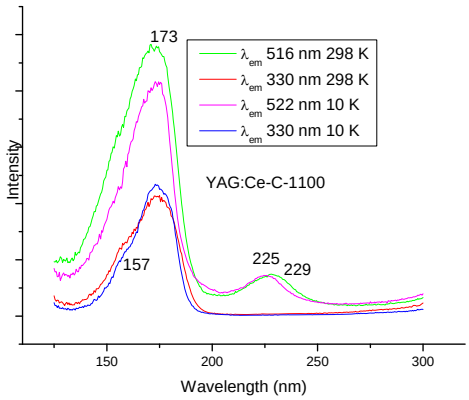

Figure 2. Synchrotron radiation excitation spectra of YAG:Ce prepared by co-precipitation synthesis and calcined at 1100 °C.

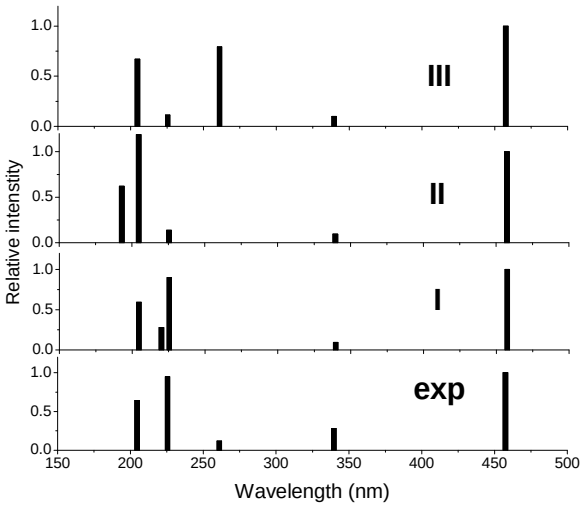

Figure 3. Schematic representations of relative intensities for 4f → 5d transitions from the the ground 4f level to excited 5d levels of YAG:Ce^{3+}. The theoretical intensities in the upper three panels were calculated using the electronic wavefunctions derived by fitting three different sets of experimental 5d levels. The lower bar chart represents the experimental values. The peak at 261 nm is due to an impurity and scheme I is correct.