Pressure-Induced Phase Transition Study of $LiYO_2$:Eu^{3+}, Gd^{3+} Phosphor

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Abstract

Lithium metal oxides (LMO's) have emerged as promising materials for photonic applications due to their wide bandgaps and tunable luminescent properties. In this work, we investigate the spectroscopic behaviour of rare-earth-doped LMO's under high-pressure conditions. Specifically, we examine the structural and optical properties of both undoped and doped $LiYO_2$ (1% Eu^{3+} and 0.5% Gd^{3+}) under ambient, low-temperature, and high-pressure conditions. The phosphor samples were synthesised using a modified Pechini method [1].

The oxide phosphors were comprehensively characterised using a range of techniques, including ambient- and high-pressure X-ray diffraction (XRD), differential scanning calorimetry (DSC), photoluminescence spectroscopy, luminescence decay measurements, and high-pressure luminescence studies employing diamond anvil cells (DAC). Initially, the samples were characterised using XRD and photoluminescence at ambient conditions to determine their structural and optical properties. Ambient-pressure XRD results revealed that the undoped sample was predominantly α-$LiYO_2$ (tetragonal, *I41/amd*) phase; however, the doped sample consisted of a mixture of both α-$LiYO_2$ (tetragonal, *I41/amd*) and β-$LiYO_2$ (monoclinic, *P21/c*) phases. Additionally, a minor fraction of cubic Y_2O_3 impurity phase was also observed in both samples. DSC analysis revealed a temperature-dependent phase transition from β-$LiYO_2$ to α-$LiYO_2$ near room temperature.

Pressure-induced phase transition studies of both samples were carried out using in situ experiments in diamond anvil cell (DAC), including synchrotron high-pressure XRD and high-pressure luminescence measurements. These results indicated a phase transition above 5.2 GPa, providing experimental evidence for a previously unreported high-pressure polymorph of $LiYO_2$, in addition to its well-known high-temperature α-$LiYO_2$ and low-temperature β-$LiYO_2$ phases.

1. L. Marciniak, W.M. Piotrowski, M. Szymczak, M. Drozd, V. Kinzhybalo, M. Back, customising thermometry: Optimising the operating temperature range of phase transition-based ratiometric luminescence thermometers, Chemical Engineering Journal 487 (2024) 150363. https://doi.org/10.1016/j.cej.2024.150363.