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Probing Disorder with Vibrational Spectroscopy – Characterization of Pr^{3+}-doped $Lu_{1.5}Y_{1.5}Al_{5-x}Sc_xO_{12}$ (x=0.0-2.0) Mixed Garnets with Scandium-induced Lattice Distortion

Lutetium and yttrium aluminum garnets are widely recognized commercial optical materials, valued for their outstanding chemical, thermal, and radiation stability. They are commonly used as phosphors, laser gain media, and detectors for beta, X-ray, and gamma radiation. Recently, praseodymium-doped variants have garnered particular interest due to their advantageous scintillation characteristics, including a fast response time of 20 ns and a high light yield of up to 30,000 photons/MeV, along with promising potential for thermometric applications in extreme environments. This study investigates the lattice dynamics of Pr^{3+}-doped $Lu_{1.5}Y_{1.5}Al_{5-x}Sc_xO_{12}$ (x = 0.0–2.0) garnets synthesized via the micro-pulling-down method. Results obtained from micro-Raman and IR spectroscopy are correlated and interpreted based on the symmetries of the crystal sites. The Raman maps are used to distinguish and characterize additional deformed perovskite-like phase inclusions that emerge at x = 2.0. Micro-Raman spectroscopy is also employed to spatially resolve the Pr^{3+} luminescence originating from both the bulk and the inclusions. The composition and structure of the samples were confirmed with VESUVIO and SXD instruments at the ISIS pulsed neutron and muon source, as well as with powder X-ray diffraction and energy-dispersive X-ray spectroscopy. These analyses confirmed that the substitution of Al^{3+} (VI, 0.535 Å) with larger Sc^{3+} ions (VI, 0.745 Å)—a size mismatch of approximately 0.21 Å—introduces lattice symmetry disruption at the octahedral sites, establishing a novel energy transfer pathway $Sc^{3+}{}_{e^- \to h^+} \longrightarrow Pr^{3+}$. Consequently, a significant enhancement in luminescence, especially in the near-infrared range, is observed compared to Sc-free crystals.

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