Engineering atomic size mismatch in La^{3+}, Pr^{3+} codoped $Lu_3Al_5O_{12}$ garnet single crystals for tailored structure and functional properties

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This study provided the first in-depth investigation of the effects of large dopant incompatibility (Pr^{3+} and La^{3+} ions) on the small host lattice element (Lu^{3+}) in $Lu_3Al_5O_{12}$ (LuAG) single crystal. The growth of such complex crystals from the melt presented many challenges [1]. By engineering the ionic radius ratio of RE- and M-site cations, a single-crystal phase stabilized by configurational entropy was achieved [2]. This investigation elucidated the crystallization behavior of configurationally disordered rare-earth aluminum garnet oxide $(Lu_{1-x-y}Pr_xLa_y)_3Al_5O_{12}$ from the melt and characterized its functional properties, including microstructural, optical, photoluminescence, and scintillation properties, between 5 and 300 K. Relaxation of the imposed strain energy led to local perturbations and destabilization of the garnet structure [3]. Multielemental EDS mapping, micro-Raman spectroscopy, and thermoluminescence revealed the mechanism by which atomic size mismatch drove a smooth transition from the garnet to the perovskite phase in high entropy garnets. The optical, photoluminescence, and scintillation measurements provided fundamental insights into property changes driven by incompatibility doping. The exploration of atomic incompatibility in oxide materials led to a deeper understanding of the complex processes observed in highly entropic oxide systems, facilitating the development of rational design approaches to enhance functionality.

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