Phase Transition in $Sc_{2-x}La_xGe_2O_7$ Solid Solution Ceramics

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$A_2B_2O_7$-type materials have been extensively investigated in the last decades due to their several technological applications, such as magnetic devices, drug detectors, gas sensors, materials for hydrogen storage, photocatalytical tools, substrates for immobilization of nuclear waste, solid oxide fuel cells, and materials for fusion reactors. Inside this group, $Sc_2Ge_2O_7$and $La_2Ge_2O_7$represents an opportunity to better understand the rare-earth germanates. An important characteristic of these compounds is the facility to form solid solution series. Due to the flexibility of the structure, many cations can be accommodated in the lattice, thus different proportions of Sc and La can be obtained, resulting in a phase transition from monoclinic to triclinic structure when replacing $Sc^{3+}$by a larger rare earth ion La^{3+}. Forming solid solution series is a useful way to modify the properties of materials through compositional design. X-ray diffraction, Raman scattering, diffuse reflectance spectroscopy and solid-state ^{45}Sc nuclear magnetic resonance were applied to track the phase transition in $Sc_{2-x}La_xGe_2O_7$(x = 0-2) solid solutions, obtained by conventional solid-state reactions. When x= 0, the pure phase $Sc_2Ge_2O_7$is monoclinic with *C2/m* (#12) space group. Increasing $x$values, the phase transition occurs with the substitution of $Sc^{3+}$by La^{3+}ions in the chemical structure, thus the monoclinic phase becomes triclinic. When x= 2, the single phase $La_2Ge_2O_7$belongs to the triclinic *P1*(#1) space group. XRD and Raman spectroscopy results were essential to confirm the phase transformation, and gradually follow the structural changes. Compositional effects on gap energies of the solid solution series were investigated by diffuse reflectance spectroscopy, applying Kubelka-Munk theory, showing the non-linear behavior of band gaps. Solid-state ^{45}Sc NMR was applied to verify the disorder caused by the substitution of ions with different ionic radius and coordination numbers.