RIETVELD REFINEMENT OF Nd AND Pr DOPED BaY_2F_8 SINGLE CRYSTALS EMPLOYING NEUTRON POWDER DIFFRACTION PATTERNS

Mazzocchi, V.L.; Mestnik-Filho, J.; Parente, C.B.R.; Cruz, S. F. A.; Baldochi, S.L

Instituto de Pesquisas Energéticas e Nucleares (IPEN-CNEN/SP)
Av. Prof. Lineu Prestes 2242, 05508-000, São Paulo, SP, Brazil

Abstract

The compound BaY_2F_8 (BAYF) possesses great potential for use in solid-state lasers. Crystals of this material have been the focus of numerous studies regarding its spectroscopy and laser applications when doped with rare-earth (RE) elements. Single crystals were growth by the zone melting method doped with Nd and co-doped with Nd-Pr for investigation of their potential as laser medium for compact laser system. Their estructural properties were investigated by neutron diffraction. Three samples were obtained by pulverizing single crystals of BaY_2F_8 doped with 2 mol% Nd (BaYF:Nd) , 2 mol% Pr (BaYF:Pr) and 0.7 mol% Nd+0.8 mol% Pr (BaYF:Nd:Pr). Diffraction patterns of the samples were measured in the IPEN-CNEN/SP PSD Neutron Powder Diffractometer. This instrument is equipped with a position sensitive detector (PSD) and a double-bent focusing silicon monochromator. The monochromator was oriented to select a neutron beam with λ = 1.4119 Å. BaYF crystallizes in the *C*2/*m* monoclinic space group. Owing to the low symmetry of this group, measured patterns presented a high density of intensity peaks. Due to the quite good resolution of the instrument, this fact did not impair the Rietveld refinement of the samples. The data were obtained, at room temperature, in a 2θ interval ranging from 10 to 130 degrees in steps of 0.05 degree. Refinement of data was performed by using the program GSAS. A typical result is that obtained for the sample BaYF:Nd where R_P and R_{WP} resulted equal to 4.5 and 5.9% , respectively. For this and for the other two samples all structural parameters, namely cell parameters, fractional atomic coordinates, temperature parameters and occupation numbers, were refined. As expected, all samples presented a single phase with the rare-earth atoms sharing positions with the yttrium atoms.