CBECIMAT
CONGRESSO BRASILEIRO DE ENGENHARIA E CIÊNCIA DOS MATERIAIS
NATAL, 09 A 13 DE NOVEMBRO DE 2002
Universidade Federal do Rio Grande do Norte
Centro de Ciências Exatas e da Terra
Departamento de Química
Departamento de Física Teórica e Experimental

X-RAY RIETVELD ANALYSIS OF PURE AND DOPED LISALF$_6$ CRYSTALS AT DIFFERENT TEMPERATURES

V. L. Mazzocchi[1], S. L. Baldochi[1], C. B. R. Parente[1], C. O. Paiva-Santos[2], C. V. Santilli[2]
CP 11049 Pinheiros, São Paulo/SP, CEP: 05422-970 – vlmazzo@curiango.ipen.br
[1] Instituto de Pesquisas Energéticas e Nucleares – IPEN-CNEN/SP
[2] Instituto de Química, Universidade do Estado de São Paulo, campus de Araraquara

In the last decade several hexafluoroaluminates with general formula LiM'M"F_6 (M'=Sr, Ca; M"= Al, Ga) were identified as potential laser crystals. In particular, the Cr^{3+}-doped LiSrAlF_6 (Cr:LiSAF) have attracted considerable attention as a near-infrared laser gain material. One of the main problems for both growth and laser application of these colquiriite-type crystals is the anisotropy of their thermal properties. In this work the Rietveld method has been employed in the study of the behavior of the cell parameters of pure and doped LiSAF crystals, as a function of the temperature. LiSAF, Cr:LiSAF, and Ce:Na:LiSAF crystals were grown by the Czochralski method. A small part of each crystal was powdered in order to prepare samples for X-ray measurements. X-ray powder patterns were measured at room temperature, 100, 200, 300, 400, 500 and 600 °C, under vacuum. The analyses of the patterns were carried out using the program DBWS-9807a. As expected, for doped compounds *a* and *c* behave in a way similar to that of pure LiSAF. The refined lattice parameters of Ce:Na:LiSAF are larger than the corresponding refined parameters of Cr:LiSAF which, in turn, are larger than those of pure LiSAF.

Keywords: Rietveld analysis, LiSAF, Czochralski method.