ICDIM Posters

Computer modeling of the tungstates Li2WO4, La2(WO4)3 and LiLn(WO4)2

Jomar B Amaral, *Departamento de Física, Universidade Federal de Sergipe, São Cristóvão/Se, Brazil;* Anderson V S Alves, *Departamento de Física, Universidade Federal de Sergipe, São Cristóvão/Se, Brazil*;Mário E G Valerio,*Departamento de Física, Universidade Federal de Sergipe, São Cristóvão/Se, Brazil;*Jair R Moraes, *Instituto de Pesquisas Energéticas e Nucleares, IPEN – CNEN/SP, Sao Paulo/SP, Brazil*;Sônia L Baldochi, *Instituto de Pesquisas Energéticas e Nucleares, IPEN – CNEN/SP, Sao Paulo/SP, Brazil*;Robert A Jackson, *School of Physical and Geographical Sciences, Keele University, Keele, Staffs ST5 5BG, UK*

jomar_amaral@yahoo.com.br

Since the discovery of X-rays by Roentgen, tungstates have mainly been used as scintillators and hosts for solid state lasers, especially when trivalent rare earth ions are incorporated as dopants. Using static computer modeling that is based on lattice energy minimization we have simulated intrinsic and extrinsic defects in the following crystal matrices: Li2WO4 (LiW), La2(WO4)3 (LaW) and LiLn(WO4)2, (LiLnW with Ln= a trivalent rare earth). The first step in the modeling procedure was to develop a set of potential parameters to describe the whole series, the simple MWO4 tungstates (M = Ca, Sr, Ba and Pb), the precursors oxides and the dopant oxides. For Eu3+ doped LiLaW at different concentrations ranging from 0.5 to 100% doping, XRD patterns and optical emission spectra have been simulated and compared with experimental data (1). Raman spectra have also been simulated and compared with CaWO4, since LiLaW has the same crystalline structure as CaWO4 with Li and La randomly distributed in the Ca sites. The defect solution energies indicates the following: i- for LiW, Li2O pseudo Schottky is the most likely among all possible intrinsic defects and the migration of Li is favored in this compound; ii- for LaW, oxygen Frenkel defects gave the lowest solution energy and the rare earth ions are expected to substitute at the La site. (1) G. Blasser, Chem. Mater., 6, 1465-1475, (1994) (2) J. R. de Moraes, S. L. Baldochi et. al., Mater. Res. Bulletin 47 (3) (2012) 744-749.