Substitutional and Interstitial Inclusions of Mn Additivies onto the KDP Lattice

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In this work, pure and Mn^{3+} doped potassium di-hydrogen phosphate (KDP and KDP:Mn) were studied through Rutherford back-scattering (RBS), Rietveld refinement (RR) and X-ray n-beam diffraction (nBD). RBS results allows the determination of KDP:Mn stoichometric formulae as $KH_2PO_{3.8}Mn_{0.4}$ while, from the RR results, it was possible to determine that the Mn^{3+} atoms are substitutional to the K ones. The lattice parameters were determined for both pure and KDP:Mn by using RR and nBD and, besides agreeing very well, they indicate the better accuracy of the results from nBD. This fact comes from the high sensitivity of the nBD technique in determine micro-crystallographic variation. According to the lattice parameter results, all values for KDP:Mn are smaller than those for KDP. Those results are also compared with a previous one, were it was determined that Mn^{3+} in concentration of 2-5 x 10^{-4} mol are occupying interstitial sites [1] and located 0.66 from (200) plane and 0.21 from (112) plane [2]. Rietveld refinement was performed from X-ray high-accuracy single crystal measurement and the nBD measurements were carried out at beam line XRD1 of the Brazilian Synchrotron Light Laboratory. All samples were grown at the same pH of 1.5.

[1] Lai X., Roberts K. J., Avanci L. H., Cardoso L. P., Sasaki J. M., *J. Appl. Cryst.*, 2003, **36**, 1230-1235. [2] Lai X., Roberts K. J., Sasaki J. M., Cardoso L. P., Bedzyk M., Lyman P. F., 2005, *in preparation*.

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