Growth and Structural Investigations on lead-doped $NdMnO_3$ Single Crystals

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Single crystals of $Nd_{(1-x)}Pb_{(x)}MnO_3$ with different dopant concentrations were grown by high temperature solution growth technique using $PbO\text{-}PbF_2$ flux [1]. Electron diffraction patterns showed the presence of superlattice structure x =0.25 and above The structure of $Nd_{(1-x)}Pb_{(x)}MnO_3$ crystals were determined by single crystal x-ray diffraction for two different x values using a Bruker AXS Smart Apex CCD diffractomenter with MoKα radiation . Positional co-ordinates of Nd and Mn atoms were obtained by SHELXS97 and refined by SHELXL97. Substitution of Pb at Nd site results in structural change from tetragonal (x=0.25) to cubic (x=0.38) lattice. The lattice parameters of tetragonal and cubic unit cells are a = b = 7.725(1)Å, c= 3.884(1) Å and a= b= c= 7.737(2) Å respectively. While the unit cell volume of tetragonal structure (*P4/mmm*) is comparable to that of parent $NdMnO_3$, the volume of cubic unit cell (*Pm3m*) is doubled. The static distortion of MnO_6 octahedra is maximum for parent orthorhombic $NdMnO_3$ (x = 0). The mismatch between different Mn - O bond lengths of $Nd_{1-x}Pb_xMnO_3$ is much less at x = 0.25 and 0.38. The MnO_6 octahedral distortion and inter octahedral tilt are removed progressively with higher doping. Changes in transport properties as a function of temperature at different doping levels are in accordance with the structural changes.

[1] Ghosh N., Elizabeth S., Bhat H.L., Subanna G.N., Sahana M., *Journal of Magnetism and Magnetic Materials*, 2003, **256**, 286-292.

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