Search for Polarons in $Li_{1-5x} Nb_{1-4x} O_{3-y}$. Structural Investigation of

the Defect Structure in Thermally Reduced Single Crystals <u>Jürg Schefer</u>^a, Dominik Schaniel^b, Theo Woike^b, Manfred Wöhlecke^c, Mirco Imlauf^c, ^aLaboratory for Neutron Scattering, ETH Zürich & PSI, CH-5232 Villigen PSI, Switzerland. ^bInstitut für Mineralogie, University at Cologne, DE-50674 K"oln, Germany. Fachbereich Physik, University of DE-49069 Osnabr["]uck, Osnabrück, Germany. E-mail: Jurg.Schefer@psi.ch

In the search for new complex materials for optical data storage, a main effect to understand is the refraction index. A bigger refraction index separarates the holograms more in space, therefore allowing a higher hologram density in the material. Interesting materials for both, application and basic understanding, are for example LiNbO3, LiTaO3 [1] and sodiumnitroprusside, Na2[Fe(CN)5NO)]2H2O [2].

 $Li_{1-5x}Nb_{1-4x}O_{3-y}$ is a widely used material. We are introducing polarons by removing oxygen in order to tune the refraction index. Neutron single crystal diffraction (TriCS, SINQ) has been used in order to determine the structural changes, mostly the determination of the removed oxygen. The results are needed in order to calculate the polaron density. We report on the defect structure of single crystals exposed to vacuum for 24h at 800°C.

[1] Strehlow W.H., et al., J. Opt. Soc., 1974, 64, 543. [2] Schaniel D., Schefer J., Delley B., Imlau M., Woike Th., Phys. Rev. B, 2002, 68, 104108. Keywords: optical materials, neutron diffraction, polarons