MS16-P10 | $LiTaO_3$ DEFECT STRUCTURES BY MEANS OF FORBIDDEN REFLECTIONS

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A wide range of optical and electrical applications of lithium tantalate $LiTaO_3$ (LTO) is closely related to its defect chemistry. Most of the defects are correlated with Li deficiency in congruent $Li_{1-5x}Ta_{5x}O_3$ (C-LTO). Near stoichiometric (NST-LTO) samples can be grown by the double-crucible Czoshralski method with larger effort. Here, we present an investigation of C- and NST-LTO in dependence of temperature using *Resonant X-ray Diffraction* (RXD) at "forbidden" reflections, giving insights into their defect chemistry. In literature, several intrinsic defect models have been suggested [10.1103/PhysRevMaterials.2.013804], which will be correlated with the energy and azimuthal dependence of the RXD.

Resonant X-ray diffraction offers powerful characterization techniques to study atomic displacements [10.1038/s41467-017-02599-6] and the local electronic structure of selected atomic positions in crystals [10.1002/crat.201300430]. In particular spectra of "forbidden" reflections only exist in the vicinity of absorption edges due to the anisotropy of electronic transitions. These "forbidden" reflections are highly sensitive to displacements of the resonant atom and, hence, to defects and vibrations. Temperature dependence allows for separation of contributions to the reflection intensity induced by thermal motion and by point defects. The obtained spectra can be modelled from first principles, using the structural information of stoichiometric LTO lattice and defect models. The "forbidden" reflections of stoichiometric LTO have no contributions of the electronic dipole transitions, therefore transitions of higher order need to be considered, the calculation of which are theoretically highly sophisticated. For instance, FDMNES can calculate these contributions and, hence, allows the numeric modelling of the experimental data.