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IDENTIFICATION OF THE DEFECT CLUSTERS IN CONGRUENT LITHIUM TANTALATE

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The combination of the extraordinary physical properties of lithium tantalate LiTaO3 (LT) offers a great potential for applications in modern optics and photovoltaics. A large fraction of such applications is based the defect chemistry. The congruently grown composition of LT using the Czochralsky method yields the cation concentration ratios of [Li]/[Ta]=48.75/51.25. Li deficiency suggests several possible configurations of a defect cluster in congruent crystals, which guarantee charge neutrality. Several intrinsic defect models have been considered in literature over several decades. Here, using a combinational approach based on DFT and solid-state NMR, we demonstrate that distribution of electric field gradients (EFGs) on a 7Li site may be regarded as a fingerprint of a specific defect configuration. The defect structure in one of two congruent LT crystals after annealing was identified experimentally and proved by the defect formation energy consideration. We found that the defect cluster in this crystal corresponded to the empty site model. The identification of the defect structure in the second LT sample was more challenging, implying the presence of extrinsic defects and an inhomogeneous defect distribution. After thermal treatment, hydrogen out-diffusion and homogeneous distribution of other defects in both LT samples were observed in the NMR and FTIR spectra. The approach of searching for the EFG fingerprints from DFT calculations in NMR spectra can be applied for identification of the defect clusters in other complex oxides.

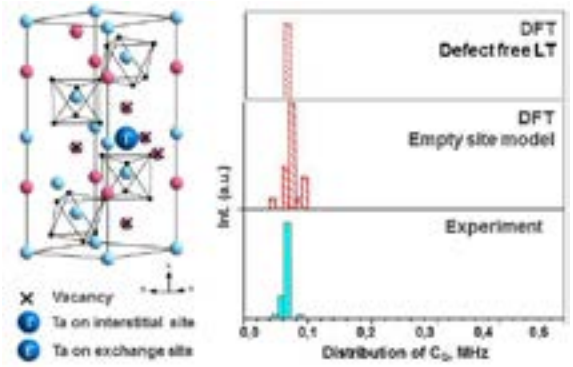

Figure. Left panel: Crystal structure of empty site defect model for non-stoichiometric lithium tantalate. Crosses and large dark blue spheres denote modified atom as compared to defect-free structure. Right panel: Classification of calculated quadrupolar coupling constants C_Q for defect-free and empty site defect models, and for experimental quadrupolar coupling constants in lithium tantalate crystal.

Recent Publications

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2. A. Vyalikh, M. Zschornak, Th. Köhler, M. Nentwich, T. Weigel, J. Hanzig, R. Zaripov, E. Vavilova, S. Gemming, E. Brendler, D.C. Meyer (2018) Analysis of the defect clusters in congruent lithium tantalate. Phys. Rev.

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Biography

Anastasia Vyalykh is a research group leader at the Technical University Bergakademie Freiberg since 2014. She received her Master degree in physics at the State University Saint-Petersburg (1999). As PhD in physical chemistry (Free University of Berlin, 2005) she focuses on the application of solid-state NMR and quantum-chemical calculations for structure determination in functional oxides, solid ionic conductors, low-dimensional carbon materials. Current research interests include studies of interfacial phenomena in organic - inorganic nanocomposites, conducting glass-ceramics, carbon-based nanohybrids as well as implementation of the in-situ methods for studies of electrochemical processes. (orcid.org/0000-0003-2326-8889).

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