Impurity locations and mechanisms of charge compensation in stoichiometric lithium niobate and lithium tantalate crystals

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Fantastic achievements in electronics have been based on detailed knowledge of impurity ions in Silicon. Therefore, tailoring properties of optical materials demands fundamental study of impurity defects. Due to very high sensitivity and resolution the radiospectroscopic methods, Electron Paramagnetic Resonance (EPR) and Electron Nuclear Double Resonance (ENDOR) allows us to obtain detailed characteristics of these defects on the atomic level. The tremendous narrowing of spectral lines found in stoichiometric crystals significantly increases the accuracy of obtainable data and, consequently, the reliability of derived models.

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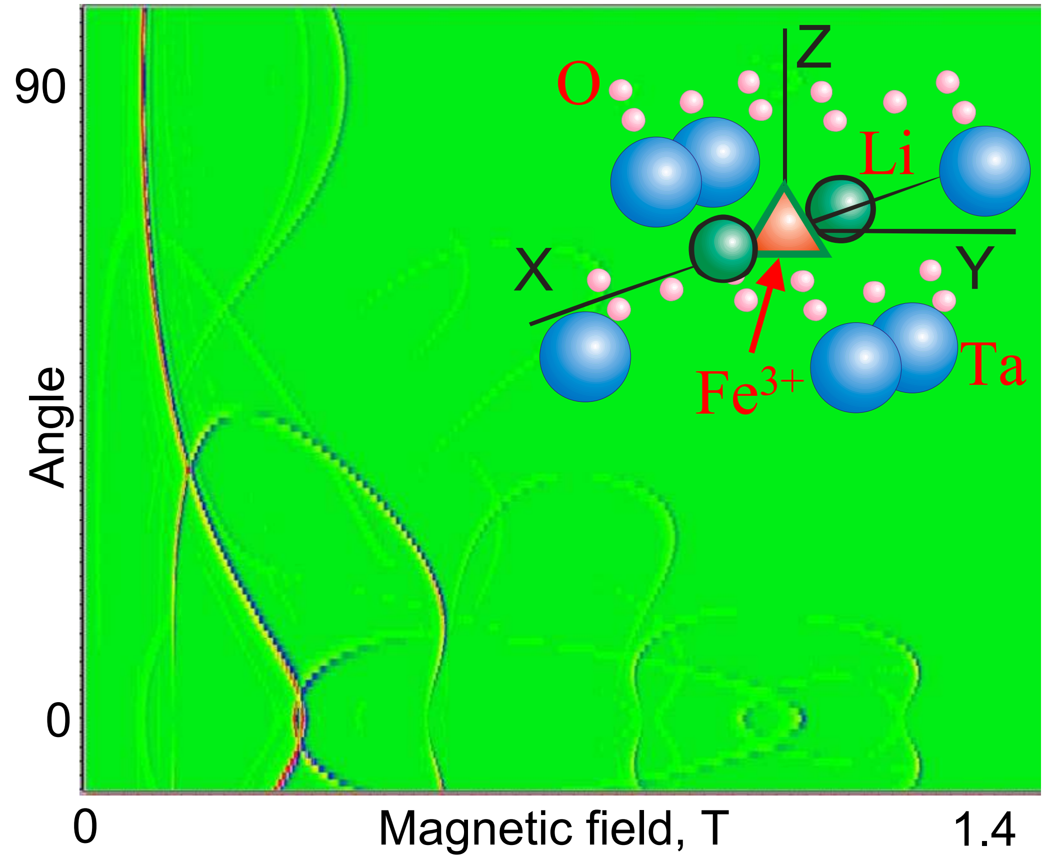

Angular dependence of the EPR spectra of stoichiometric $LiTaO_3$ crystal doped with iron (measured by R.Petersen) and a model of the Fe^{3+} center derived from the EPR/ENDOR data.

It is well known that impurities and intrinsic defects in materials can be harmful or useful. Knowledge of the defect structure and influence of the defect on material properties allows us to obtain material with desirable characteristics. For instance, intentional doping of super-pure Silicon with very small amount of Phosphorus or Boron (about 1 atom per million) changes drastically a conductivity of the material, and this is widely used for the construction of diodes and transistors for computer processors and graphic cards. The basis for today achievements in electronics was created by fundamental investigations of intrinsic and extrinsic defects in Si, made about 50 years ago.

Using light instead of electrons promises essential increase of the operation speed of elements and devices for optical telecommunication, optical computers and so on, since light speed exceeds thousands times the speed of electrons. Lithium niobate and lithium tantalate crystals are considered as the most viable candidates for “one material technology platform” for all-optical telecommunication network.

The identification of the main crystal defects on the atomic level is a huge and difficult work. However, it has to be done for optical materials too. Our group investigates impurity locations and mechanisms of charge compensation with the help of magnetic resonance methods. Main part of the work is conducted at the Bozeman campus of Montana State University with the collaboration with our partners from Germany, Armenia and Ukraine.

The conventional lithium niobate crystals are grown from a Li-deficient congruent melt, and therefore, they have a great concentration of intrinsic defects (like non-purified Silicon). This causes to strong broadening of all spectral lines, and hampers the study of fine physical effects. Our group found possibilities to obtain defects free stoichiometric materials with 10-20 times narrower spectral lines. The tremendous line narrowing significantly increases the accuracy of obtainable data and, consequently, the reliability of derived models. Moreover, we found that crystals with reduced concentration of intrinsic defects have essentially different properties in comparison with conventional materials, and that for special applications the characteristics of stoichiometric crystals are often better than congruent ones. During last year (the project started in August 2003) thousand spectra were recorded and many new results were already obtained. These achievements were presented on several national and international conferences: *APS meeting*, Montreal, Canada, 2004; *47th Rocky Mountain Conference on Analytical Chemistry*, Denver, USA, 2004; *International Conference on Defects in Insulating Materials (ICDIM)*, Riga, Latvia, 2004 (invited key-note talk). They were accepted by scientific community with a very great interest.

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Education:

Three undergraduates (Ben Losby, Mark Munro, and Robert Petersen), and two research scientists (Valentin Grachev and Viktor Bratus) contributed to this work.

Robert Petersen received a MSU Undergraduate Scholars Program award for 2003-2004, as well as a MSU REU Site Program scholarship for Summer 2003; Ben Losby received a MSU REU Site Program scholarship for Summer 2004. This summer, 2004, both Munro and Petersen work in our laboratory thanks to a NSF supplement to the main grant. At present all students operate successfully with our complex spectroscopic technique.

The PI and students prepare our Bruker ELEXSYS 560 spectrometer for measurements of magnetic resonance at liquid helium temperature.