TRACE IMPURITIES, INTRINSIC AND RADIATION DEFECTS IN OXIDE MATERIALS

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Solar, cosmic, laser or nuclear reactor radiations lead to the appearance of defects in complex oxides and to inevitable performance degradation of devices based on these materials. The study of non-controllable (trace) impurities, intrinsic and radiation defects is the only way of understanding degradation mechanisms. Since most of point defects are paramagnetic, the high sensitive Electron Paramagnetic Resonance (EPR) is the most suitable method for their study. The present work reports the EPR and simultaneous EPR/optical study of defects in single crystals irradiated by gamma photons, electrons, protons and neutrons. Among investigated oxide materials are $LiNbO_3$, $Li_2B_4O_7$, $KTiOPO_4$, and $Ba_{0.77}Ca_{0.23}TiO_3$. The oxide crystals from different vendors or grown by different ways have usually different concentrations of non-controllable impurities and, as a result, different physical properties. For instance, there are many EPR lines of non-controlled impurities in $KTiOPO_4$ crystals. However, since these lines are rather narrow, these crystals do not have intrinsic defects like vacancies and antisites, which dominate in non-stoichiometric crystals like congruent lithium niobate. As-grown non-irradiated $Li_2B_4O_7$ samples give no visible EPR signals. It means that the samples have a very good quality and no impurities in paramagnetic state. We did not find also a significant EPR signal in the samples after gamma-irradiation, which usually produces electrons and holes. We have to conclude that defects, which could capture electrons or holes, as well as impurities, which could be recharged to paramagnetic state are practically absent. However, strong EPR signals appeared after neutron irradiation. Analyzing data obtained in our lab, as well as published data, we came to the conclusion that all observed radiation defects in oxide crystals can be divided into six basic groups: (1) Recharged impurity ions, (2) Recharged regular lattice ions near intrinsic or extrinsic lattice defects, like O^- centers (hole traps) or Ti^{3+} (electron traps), (3) F-like centers with $g \approx 2.00$ representing an electron trapped by an oxygen vacancy, (4) Centers in the form of the O^0 - O^- (or O_2^-) complex consisting of two oxygen ions in regular sites near a metal vacancy (hole traps), (5) The O^0 - O^- complex consisting of one regular site oxygen and one interstitial oxygen (hole traps), (6) Recharged ions knocked out from their regular lattice sites. The dominating types of defects formed under visible, UV and gamma photon irradiation are centers created by defects trapped electron or hole (groups 1-4). The neutron and high energy electron irradiation creates stable Frenkel pairs - interstitial ions and vacancies (groups 3-6). The obtained data about radiation defects can be used for a preliminary selection of materials and samples suitable for various applications. The research was supported by NASA.