Forbidden reflections induced by unit-cell elastic distortions in paratellurite crystals

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Paratellurite TeO_2 crystals under the application of a strong electric field demonstrate significant changes of the shape of allowed reflections, which are associated with the migration of oxygen vacancies to the surface layers [1]. Similar effect was found earlier in strontium titanate SrTiO₃ and got the name of "migration-induced field-stabilized polar phase" [2].

An experiment was carried out at P23 beamline of PETRA III synchrotron, devoted to the study of the changes in the forbidden reflections 002 and 100 in TeO₂ under applied electric field. These reflections are forbidden in conventional X-ray scattering, but can be observed at the energies close to absorption L-edges of Te, due to appearance of dipole-dipole resonant contribution to the atomic factor of Te. The experiment was carried out at the incident radiation energy, close to L_1 edge of Te 4938 eV. For both reflections the azimuthal dependence and energy spectrum were measured with and without application of electric field. For 002 reflection electric field magnitude was 500 and 750 V/mm, for 100 reflection it was 750 and 1050 V/mm.

We have observed a change of azimuthal dependence (Fig.1) caused by the violation of a symmetry in electric field in accordance with the predictions of preliminary theoretical calculations. Also we have observed a change of the energy spectrum at the field magnitude of 500 V/mm. It is assumed that this change is caused by appearance of oxygen vacancies in the environment of Te. For reflection 100 this change of the energy spectrum was even more obvious. This is justified because in this experimental geometry migration of vacancies is more pronounced.

1,0



0.8 0.6 0.6 0.6 0.2 0.0 4920 4920 4940 4960 4960 4980 5000 Energy (eV)

TeO₂, 002

E=0 V/mm

E=750 V/mr

Fig.1. The azimuthal dependence of the 002 reflection at 4938 eV without (black) and with electic field (red and green).

Fig.2. Energy spectrum of the 002 reflection without (black) and with electric field (red).

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