Thin layer formation in TeO_2 single crystals due to migration of charge carriers

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Currently, a significant area of materials science concerns the development of mechanisms for controlled variation of a material's structure through local defects formation. This ensures the adjustment of a material's structural organization and functional properties for application in novel data storages, sensors, and energy accumulation systems, among others.

The near-surface structural variation has been found in $SrTiO_3$ [1] and in TeO_2 single crystals as well. It is caused by the migration of oxygen vacancies in an external electric field. The dynamics and anisotropy of the formation process of near-surface structures in paratellurite (α-TeO_2) single crystals due to the migration of charge carriers induced by an external electric field are studied by the *in-situ* X-ray diffraction (XRD) technique and electrical conductivity measurements.

Single crystal diffraction patterns exhibit an interesting response on an external electric field. The observed effect manifests itself in the diffraction rocking curve (DRC) parameters and its shape variation with a reversible character [2]. This is explained by the formation of the strain field (domains) with a small mutual angular misorientation. The threshold field strength about 100 V/mm, above which the broadening of the XRD reflection peak starts, has been revealed. A linear dependence of the broadening value on the applied field strength has been determined.

A diffraction peak broadening occurs for both polarities with a simultaneous shift of its maximum only occurring on the surface with a positive electric potential [3]. For the (110) crystal cut, a much higher saturation time (800-1000 s) of the process compared to the (100) cut (~300 s) is registered. Moreover, in all cases, the relaxation is almost 2–3 times faster than the saturation, thereby repeating the character of the measured electrical conductivity. The electric field application along the fourth-order axis [001] doesn't lead to visible changes in the diffraction peak parameters.

A thickness of the layer with a strain formed close to the surface is estimated by XRD at different diffraction orders [4]. The experimental data is compared with the results of DRC simulation considering the crystal lattice deformation with the depth attenuation. The simulation shows the strain localization depth of 3.6 μm for the (110) crystallographic cut, whereas the diffraction peak profile for the (100) cut is suitably described by a layer with a thickness of 1.6 μm.

Calculation according to the electrical measurements shows that the Debye screening layer of charge is localized at the same characteristic length. The concentration of defects in the near-surface region is inversely dependent on the screening length and reaches the value of 1.3×10^{22} m^{-3}, which is three orders of magnitude greater than vacancies concentration in the bulk.

[1] Hanzig, J., Zschornak, M., Hanzig, F., Mehner, E., Stöcker, H., Abendroth, B., Röder, C., Talkenberger, A., Schreiber, G., Rafaja, D., Gemming, S., & Meyer D. C. (2013). Physical Review B 88, 024104.

[2] Kovalchuk, M. V., Blagov, A. E., Kulikov, A. G., Marchenkov, N. V. & Pisarevsky, Yu. V. (2014). Crystallography Reports 59(6), 862.

[3] Kulikov, A. G., Blagov, A. E., Marchenkov, N. V., Lomonov, V. A., Vinogradov, A. V., Pisarevsky, Yu. V. & Kovalchuk, M. V. (2018). JETP Letters 107(10), 646.

[4] Kulikov, A. G., Blagov, A. E., Ilin, A. S., Marchenkov, N. V., Pisarevsky, Yu. V. & Kovalchuk, M. V. (2020). Journal of Applied Physics 127, 065106.

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