Analysis of Electromigration in MWO₄ (M=Ca, Cd, Pb, Zn) Crystals and their Structural Defects

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The complex oxide crystals characterized by mixed electron-ionic conductivity. The electrical properties and migration of charge carriers of some oxide compounds were investigated previous in connection with the structural building and electrical active defects of crystals in our papers [1, 2]. However, the electrical properties of AWO₄ (where A is Ca, Cd, Pb, or Zn) were studied insufficiently. In the book [3] the data on ionic conductivity of crystals of different structural types based on the crystallographic characteristics are given. The effect of migration of tungstate complexes at high temperatures for CaWO₄ crystal was observed in [4]. The ionic conductivity of crystals with scheelite type of structure experimentally investigated [5] in PbWO₄ and PbMoO₄ compounds. But, the mechanism of ionic conductivity and the migration ways of mobile ions in these crystals are not ascertained.

In this work the stereo-atomic crystal structure analysis using the program package TOPOS [6, 7], with the aim to visualization of probable migration pathway of mobile ion in the crystals with general formula AWO₄ (A=Ca, Cd, Pb, or Zn) was applied. The ionic migration maps for the crystals AWO₄ were constructed. Possible migration paths of W ions in the structure of the AWO₄ crystals with scheelite (Ca, Pb, space group I4₁/a) and wolframite (Cd, Zn, space group P2₁/c) structure types at different temperatures (room and higher) were analyzed. Consideration of chemical and structural factors and visualization of conduction pathways are promoted the determination of mechanisms and other spatial features of ions migration in crystals. This approach allowed also the forecast of crystal properties and applications. The some basic concepts on micro-level investigation of the mobile ion migrations in crystal lattice and previous results of calculations were considered in our works [8-10].

We show the mobility of W ions in the crystals AWO₄. The obtained results were applied to design of structural defects. The own point defects are considered. In particular the plurality of the WO₄²⁻ oxy-anion as known basic luminescent centers in AWO₄ crystals was motivated.