Analysis of Electromigration in MWO_4 (M=Ca, Cd, Pb, Zn) Crystals and their Structural Defects

V.N. Shevchuk*, I.V. Kayun

Department of Electronics and Computational Technologies,
Ivan Franko National University of Lviv, 50 Drahomanov Street, 79005 Lviv, Ukraine
** shevchuk@electronics.lnu.edu.ua*

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 AWO_4 (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 $CaWO_4$ crystal was observed in [4]. The ionic conductivity of crystals with scheelite type of structure experimentally investigated [5] in $PbWO_4$ and $PbMoO_4$ 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 AWO_4 (A=Ca, Cd, Pb, or Zn) was applied. The ionic migration maps for the crystals AWO_4 were constructed. Possible migration paths of W ions in the structure of the AWO_4 crystals with scheelite (Ca, Pb, space group $I4_1/a$) and wolframite (Cd, Zn, space group $P2/c$) 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 AWO_4. The obtained results were applied to design of structural defects. The own point defects are considered. In particular the plurality of the WO_4^{2-} oxy-anion as known basic luminescent centers in AWO_4 crystals was motivated.

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