MODELING OF THE PROCESSES OF IONIC CONDUCTIVITY IN A SOLID OXIDE ELECTROLYTE BASED ON ZrO_2

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Currently, in connection with scientific and applied research in the search for alternative energy sources and increasing the efficiency of known sources, the study of solid oxide fuel cells (SOFC) is an urgent task of modern physics and chemistry. The main components of the SOFC are anode, cathode and electrolyte. As the anode material, cermet is often used from nickel and solid oxide electrolyte, and lanthanum-strontium manganite compounds are used as the cathode.

It is known, that solid oxide fuel cells (SOFCs) are more effective among alternative energy sources. For such qualities as efficiency, environmental friendliness, fuel quality and noise level in the production of electricity, SOFCs are more efficient than other sources of electricity. In SOFC, natural gas, methane, butane, propane, etc. can be used as fuel. The use of hydrogen as a fuel makes SOFC more environmentally attractive. In this case, emitted into the atmosphere water vapor, which is formed during the electrooxidation of hydrogen. Pure oxygen or air is an oxidizer in SOFC. Oxygen is reduced to ions, which are transported through the oxygen vacancies of the crystal lattice of the solid electrolyte and react at the anode with hydrogen to form water. In order for these reactions to occur, the anode and cathode must be connected to the load. Then an electric current flows through the external circuit.

At present, the search continues for mechanically strong new oxide materials with anionic conductivity. It is known that a nanostructured oxide ceramics based on ZrO_2 possesses increased physical and chemical properties compared to ceramics obtained by commonly used industrial methods or by solid-phase synthesis. If metal impurities with a lower valence are introduced into zirconia, they will usually occupy cationic sites. In this case, oxygen ions leave the lattice in such a quantity that the electroneutrality condition is fulfilled. For example, if atoms of bivalent calcium are introduced, then for each introduced atom there will be one remote oxygen ion.

Modeling of the ionic conductivity processes in a solid electrolyte based on zirconia will use a package of semi-empirical quantum chemical programs MOPAC-2016 in the PM7 approximation.

We constructed a model of zirconium dioxide, consisting of 96 atoms, i.e. 32 atoms of Zr, 64 oxygen atoms corresponding to the cubic structure. The dimensions of the nanostructure under consideration were about 14, 13 and 12 angstroms, respectively, in three directions. The ionization potential is 3.553 eV. The width of the band gap, defined as the energy difference of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), was 3.2 eV. This value of the width of the forbidden band is much smaller than the experimental value, which is 6 eV.

The paper will discuss the results of quantum-chemical modeling of the migration of oxygen ions in the cubic structure of a pure crystal ZrO_2 and stabilized zirconia with CaO, MgO impurities.