Reaction fronts and ambipolar chemical diffusion in oxide crystals

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We study theoretically the impact of oxygen diffusion in oxide crystals on the dynamic changes of metal dopants in the ionic state, and on the crystal conduction type. The analysis invokes ambipolar diffusion for all participating species: oxygen vacancies, metal dopant, holes and electrons. The species dynamics are demonstrated for an oxide of 8 eV energy gap, electron and hole diffusivities being 10^5 times larger than the oxygen vacancy one, and the dopant energy level being 1.0 eV above or 1.0 eV below the mid-gap. We obtain linkage between the oxygen chemical diffusivity and the occurrence of a reaction front. The necessary condition is the existence of a sufficiently long interval, where a power dependence of the oxygen chemical diffusivity on the ambient oxygen pressure exists. In our demonstrated system, prominent reaction fronts occur at very low and at very high ambient oxygen pressures. The fronts relate to the reversible $\mathrm{M}_{\mathrm{Me}}^{\times} + \mathrm{e}' \overset{\leftarrow}{\longrightarrow} \mathrm{M}_{\mathrm{Me}}'$ reaction at the low pressures, and to the reversible $\mathrm{M}_{\mathrm{Me}}' + \mathrm{h}^{\bullet} \overset{\leftarrow}{\longrightarrow} \mathrm{M}_{\mathrm{Me}}^{\times}$ reaction at high pressures, where M marks the dopant metal, and Me marks an oxide lattice constituent metal.