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High CO_2 tolerance oxygen permeation membranes $BaFe_{0.95-x}Ca_{0.05}Ti_xO_{3-\delta}$

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Abstract: A high CO_2-tolerance oxygen permeation membrane $BaFe_{0.95-x}Ca_{0.05}Ti_xO_{3-\delta}$ (BFCT, x = 0.05-0.15) was designed and prepared. Single cubic perovskite phase can be maintained up to the doping level x = 0.15. The Ti substitution enhances significantly the CO_2 tolerance and improve the structural stability under H_2 containing atmosphere of BFCT materials. With increasing Ti doping level, the oxygen vacancy concentration decreases and the oxygen ion migration energy increases, leading to a slight decrease in oxygen permeability of BFCT materials. Nevertheless, the sample $BaFe_{0.8}Ca_{0.05}Ti_{0.15}O_{3-\delta}$ delivers a high oxygen permeation flux of 1.02 mL min^{-1} cm^{-2} at 950 ^oC for 1 mm thick membrane. The Ti substitution alleviates the lattice oxygen loss and reduces the thermal expansion coefficient of BFCT. A combination study of experimental measurements and first principles calculation was conducted to advance the understanding of Ti effects on the electrical conductivity behavior in BFCT. The BFCT membranes show an excellent long-term operation stability. The high oxygen permeability, good structural stability under CO_2 and reducing atmosphere make the BFCT (x = 0.15) a promising membrane for oxygen separation applications.

Keywords: Perovskite; Oxygen permeability; Oxygen ion migration; CO_2-tolerance ability; Structure stability.