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研究论文

Sr 取代 $LaFeO_3$ 钙钛矿的结构性质和催化性能

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摘要 Sr^{2+}对La^{3+}的部分取代导致$LaFeO_3$的结构性质和催化性能发生了显著变化. 钙钛矿结构由$LaFeO_3$的正交型变成了$La_{0.8}Sr_{0.2}FeO_3$的近立方型. 由于电荷补偿效应, Sr^{2+}取代La^{3+}导致部分Fe^{3+}氧化为Fe^{4+}, 同时产生氧空穴,因而提高了$La_{0.8}Sr_{0.2}FeO_3$的还原性能. 由于氧空穴的作用, $La_{0.8}Sr_{0.2}FeO_3$催化剂在?CO?氧化和CH_4燃烧反应中均表现出较$LaFeO_3$高的催化活性. 在CO氧化反应中, 氧空穴有利于反应物分子的吸附并加速了气相氧分子在表面上的解离; 而在CH_4燃烧反应中, 氧空穴则促进了晶格氧物种从体相到表面的扩散.

关键词: 钙钛矿 铁酸镧 取代 还原性 一氧化碳氧化 甲烷燃烧

Abstract: Partial substitution of La^{3+} by Sr^{2+} in $LaFeO_3$ resulted in significant changes in its structure and catalytic activity. The perovskite structure was changed from orthorhombic in $LaFeO_3$ to nearly cubic in $La_{0.8}Sr_{0.2}FeO_3$. Replacement of La^{3+} by Sr^{2+} induced a positive charge deficiency that was compensated for by the oxidation of some Fe^{3+} to Fe^{4+} and the generation of oxygen vacancies, which greatly promoted the reducibility of the perovskite. $La_{0.8}Sr_{0.2}FeO_3$ gave considerably enhanced activity in CO oxidation and methane combustion because the oxygen vacancies accelerated the dissociation of gaseous oxygen on the surface in CO oxidation and facilitated the diffusion of lattice oxygen from the bulk to the surface during CH_4 combustion.

Keywords: perovskite, lanthanum ferrite, substitution, reducibility, carbon monoxide oxidation, methane combustion

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