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Structural and catalytic properties of thin CeO_2 films on TiO_2 substrate I.G. BATYREV, ARL, Adelphi, MD, S.N. RASHKEEV, INL, Idaho Fals, ID — Structural properties of $CeO_2(111)$ thin films on top of a $TiO_2(110)$ substrate have been investigated by first-principles calculations. We found the special orientation of the ceria film relative to the rutile substrate that corresponds to a small (few percent) lattice mismatch between the two oxide surfaces. The positions of interfacial Ti atoms undergo some structural modulations during the relaxation process. Also, the relaxation of the interface resulted in the appearance of elongated Ce-O bonds at some sites of the O-terminated surface of CeO_2/TiO_2 films. These oxygen sites at the surface show low activation energy for loosing oxygen atoms and, therefore, they have higher catalytic activity in CO oxidation by the Mars-van Krevelen mechanism. We predict from the simulations that higher rate of the catalytic CO oxidation should have $CeO_2(111)/TiO_2(110)$ films compared with $CeO_2(111)$ surface, which may also be attributed to the elongation of Ce-O bonds at some sites of O-terminated film in comparison with a pure ceria surface. We discuss the role of oxygen vacancies in the CO oxidation at reduced films and investigate the interplay between migration of O bulk atoms to the surface O vacancy sites and the structural phase transition from the $CeO_2(111)$ (Ce^{4+}) and $Ce_2O_3(0001)$ (Ce^{3+}) structures. This work was supported by the U. S. Department of Energy Contract DE-AC07-051D14517.

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