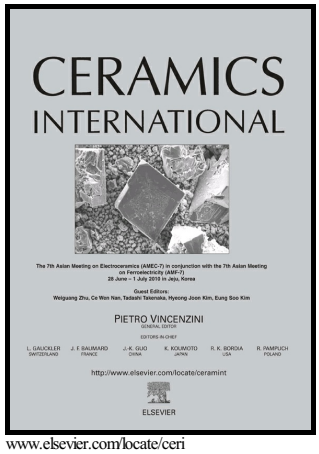

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PII: S0272-8842(18)31491-3
DOI: https://doi.org/10.1016/j.ceramint.2018.06.059
Reference: CERI18503

To appear in: *Ceramics International*

Received date: 2 April 2018
Revised date: 11 May 2018
Accepted date: 8 June 2018

Cite this article as: Hussein A. Miran, Zhong-Tao Jiang, Mohammednoor Altarawneh, Jean-Pierre Veder, Zhi-feng Zhou, M Mahbubur Rahman, Zainab N. Jaf and Bogdan Z. Dlugogorski, Influence of DC magnetron sputtering reaction gas on structural and optical characteristics of Ce-oxide thin films, *Ceramics International,* https://doi.org/10.1016/j.ceramint.2018.06.059

Influence of DC magnetron sputtering reaction gas on structural and optical characteristics of Ce-oxide thin films

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Abstract

The influence of the reaction gas composition during the DC magnetron sputtering process on the structural, chemical and optical properties of Ce-oxide thin films was investigated. X-ray diffraction (XRD) studies confirmed that all thin films exhibited a polycrystalline character with cubic fluorite structure for cerium dioxide. X-ray photoelectron spectroscopy (XPS) analyses revealed that cerium is present in two oxidation states, namely as CeO_2 and Ce_2O_3, at the surface of the films prepared at argon-oxygen flow ratios between 0-7%, whereas the films are completely oxidized into CeO_2 as the aforementioned ratio increases beyond 14%. Various optical parameters for the thin films (including an optical band gap in the range of 2.25 – 3.1 eV) were derived from the UV-Vis reflectance. A significant change in the band gap was observed as the oxygen pressure was raised from 7% to 14% and this finding is consistent with the high-resolution XPS analysis of Ce 3d that reports a mixture of Ce_2O_3 and CeO_2 in the films. Density functional theory (DFT+U) implemented in the Cambridge Serial Total Energy Package (CASTEP) was carried out to simulate the optical constants of CeO_2 clusters at ground state. The computed electronic density of states (DOSs) of the optimized unit cell of CeO_2 yields a band