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Influence of reaction gases on the structural and optical characteristics of Ce-oxide thin film coatings

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Ce-oxide thin film coatings present unique optical properties. In this study, structural, chemical bonding and optical properties of the thin films in relation to the composition of reaction gas via sputtering process were investigated. All the thin films exhibited a polycrystalline character with cubic fluorite-structure for cerium dioxide along (111), (200) and (222) orientations. XPS analysis revealed that two oxidation states of CeO_2 and Ce_2O_3 are present in the films prepared at lower argon-oxygen flow ratios, whereas the films are totally oxidized into CeO_2 as the aforementioned ratio increases. Optical parameters (α, ε1, ε2, n and k) derived from UV-Vis reflectance data indicate that the thin films have indirect optical band gaps in the range of 2.25-3.1 eV. Density Functional Theory (DFT+U) implemented in the Cambridge Serial Total Energy Package (CASTEP) has been employed to model some optical properties of CeO_2 cluster at ground state. The simulated electronic Density of State (DOS) of the relaxed structure of CeO_2 demonstrates a band gap, agrees well with the measured optical band gap. The experimental and calculated absorption coefficient (α), have analogous trends and to some extent a similar range of values in the wave length. All in all, our theoretical findings consistently support the experimental results.

Biography

Zainab N Jaf has completed her Master's degree from College of Education for Pure Sciences/Ibn Al-Haitham, Department of Physics, University of Bagdad, Iraq. She is currently pursuing her PhD degree.

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