Nanostructured Zr doped α-Fe_2O_3 Thin Films for PEC Generation of Hydrogen

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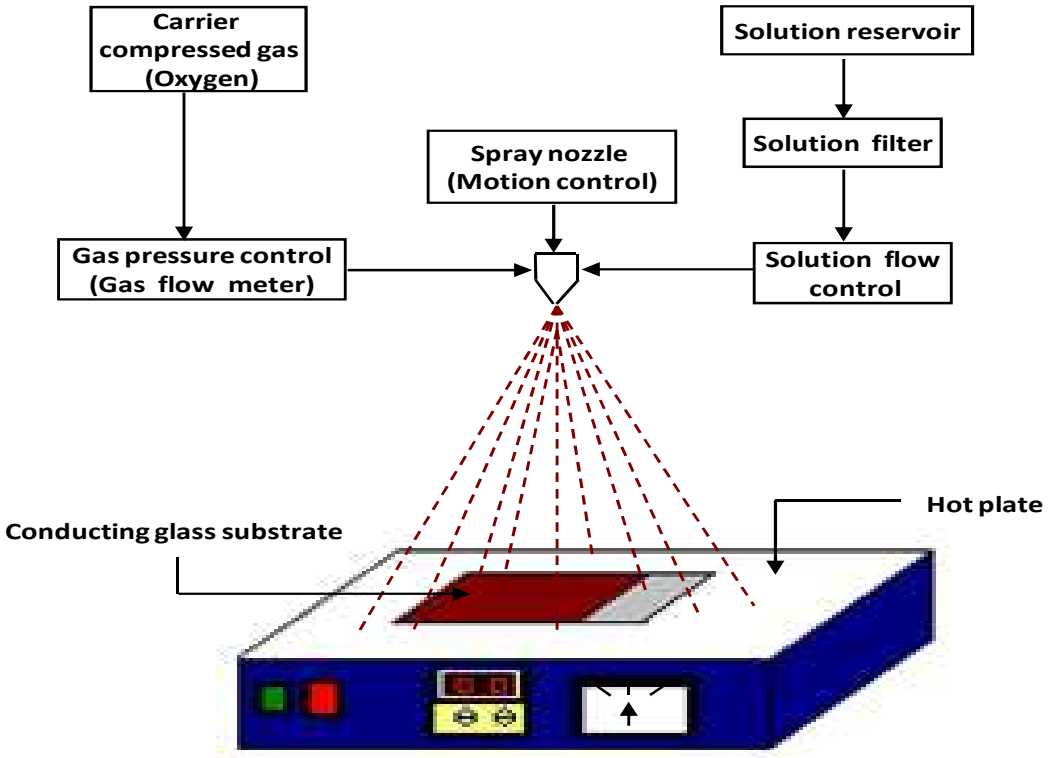
Outline

- Zr doped α-Fe_2O_3 Thin Film in PEC
- Experimental Study
  - ✓ Thin Film Preparation
  - ✓ Characterization (XRD,UV visible, SEM, XPS)
  - ✓ PEC Study (Mott-schottky, I-V Curves)
- Results/Conclusion

Thin Film Preparation

Spray Pyrolysis Unit

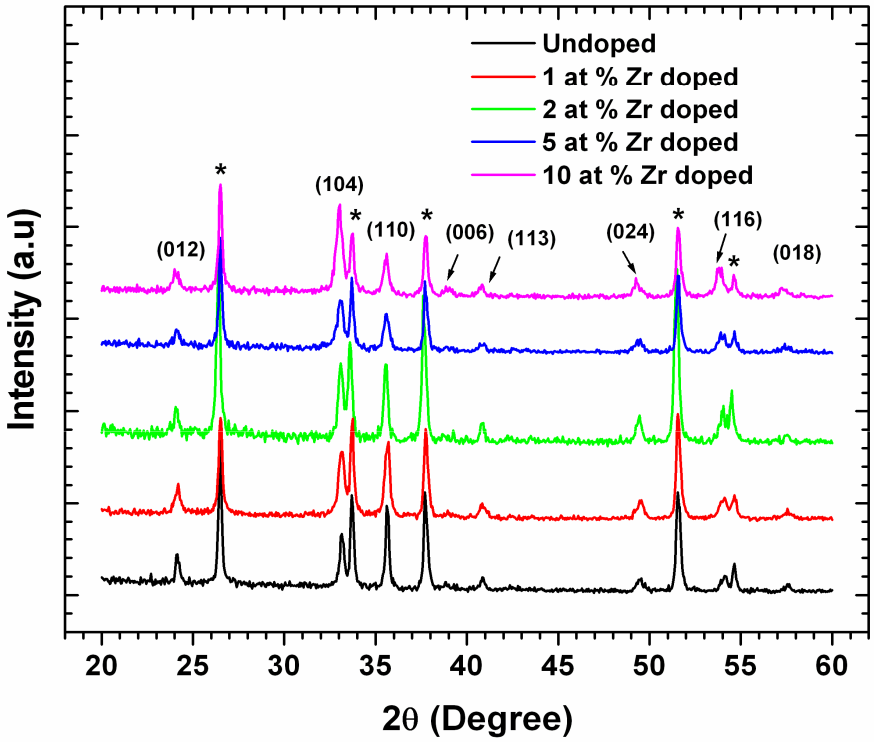


Spray Parameters	Optimal Values
Molarity of iron nitrate solution	0.15M
Substrate temperature	350 ^{o}C
Distance of nozzle from substrate	25 cm
Flow rate from burette	5.4 ml/min
Air pressure	2.0 kg/cm^2
Duration of each spray	10 sec
Total spray time	100 sec

Zr doping: 1.0, 2.0, 5.0 and 10.0 at % zirconyl chloride octahydrate was added to precursor solution

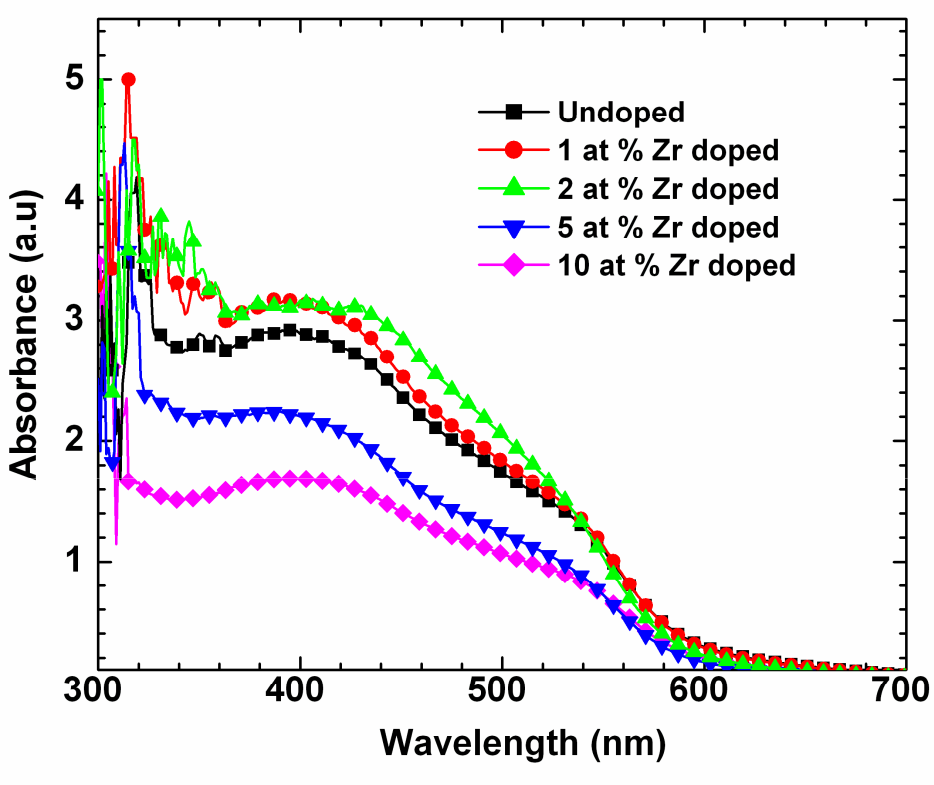
The prepared thin films were annealed in muffle furnace at 500 ^{o}C for 2 hours

X-Ray Diffraction Plots



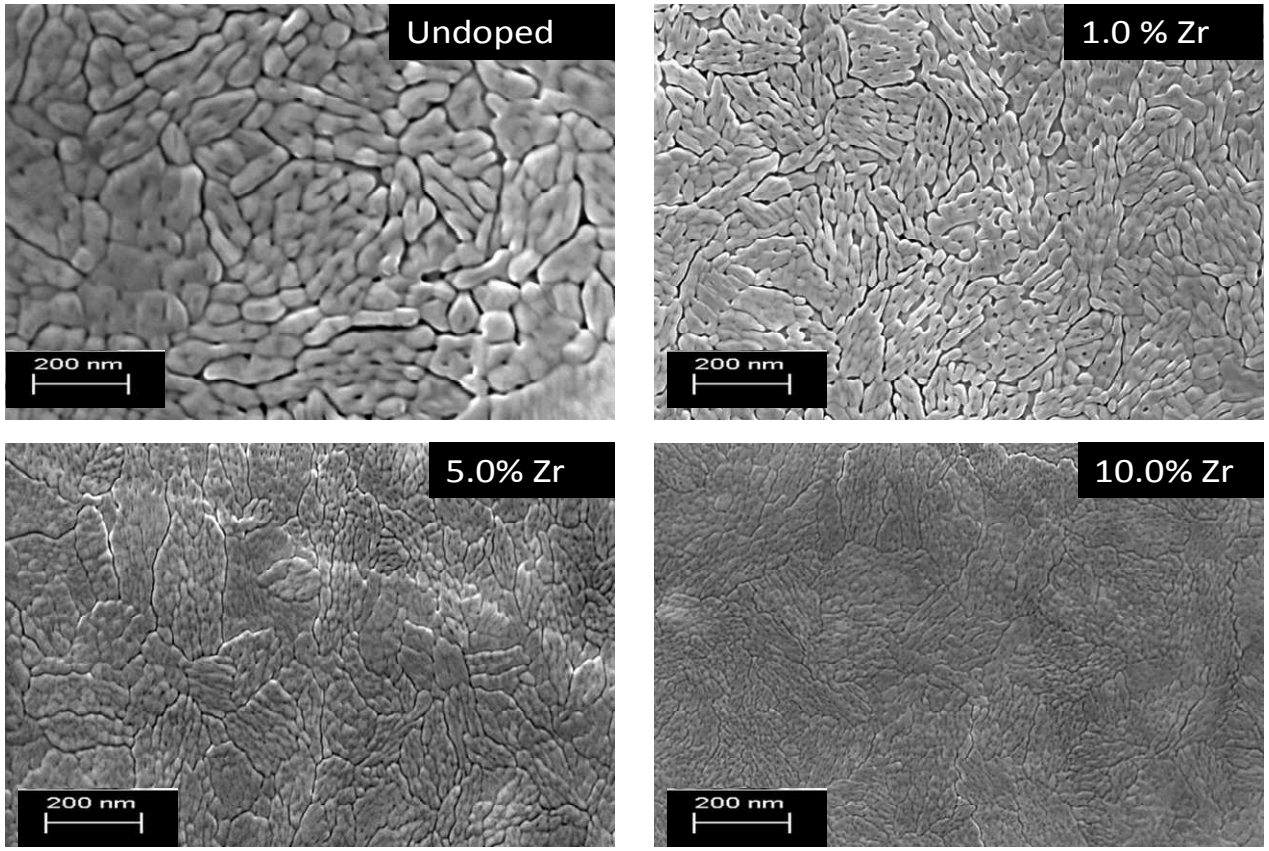
- Undoped and low concentration Zr doped thin film exhibited most intense peak at 2θ= 35.6° showing the dominance of 110 plane of α-Fe_2O_3 while at higher doping concentration intensity of peak at 2θ=33.4°, corresponding to reflection 104 started dominating.
- Average crystallite size calculate using 110 peak of XRD data decrease from ~51 nm for undoped to ~22 nm for 10.0% Zr doped α-Fe_2O_3

UV-Vis Absorption



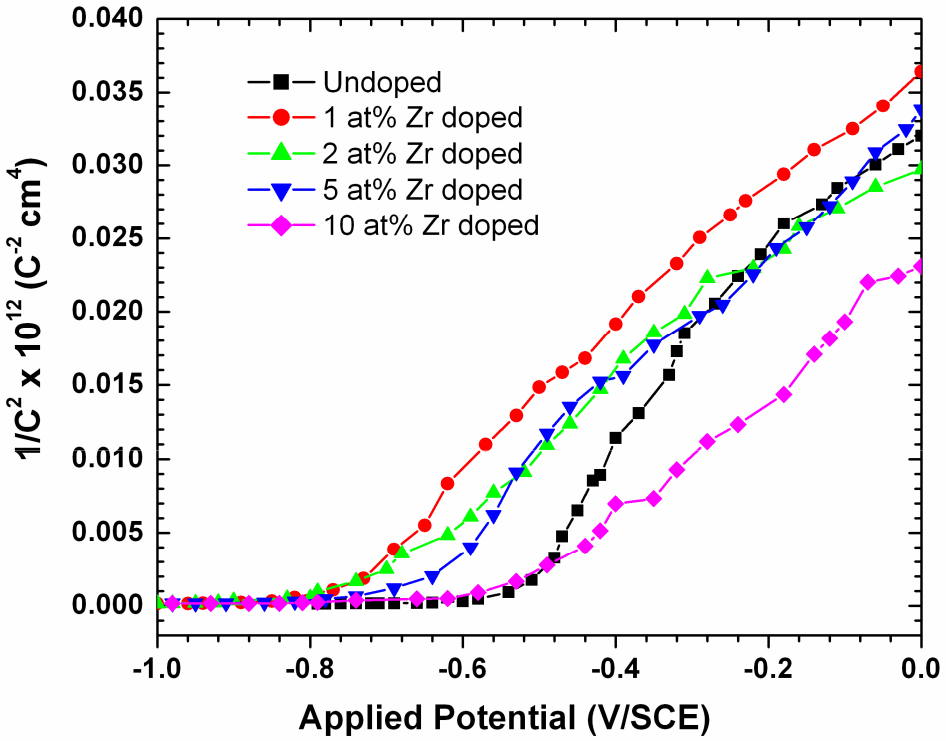
- Value of absorbance was observed to increase minutely for the samples doped with Zr at 1.0% and 2.0% doping level, but at higher concentration of doping it was found to decrease.
- The values of band gap was observed to increased from 1.9 eV for undoped to 2.0 eV for 10.0% Zr doped samples.

SEM: Morphology



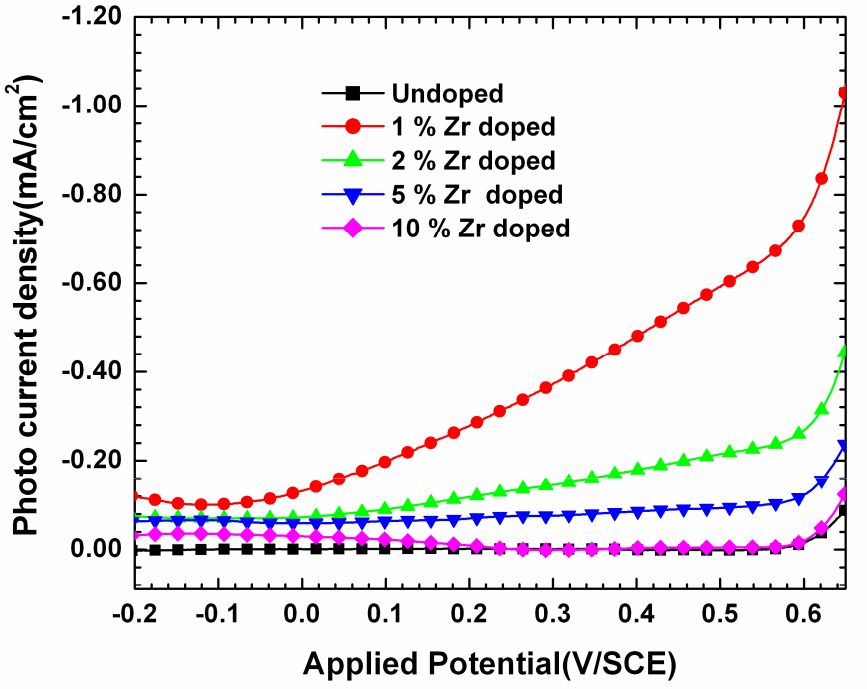
- FE-SEM images obtained for all undoped and Zr-doped α-Fe_2O_3 films exhibited porous surface structure with worm like irregular grains
- With the increase in Zr doping concentration, porosity of the film was observed to decrease, leading to the more densification of the iron oxide structure

Mott-Schottky Plots



- Flat band potential was observed to increase from -0.6 V/SCE for undoped to -0.85 V/SCE for 1.0% Zr doped sample and afterward decreased .
- Donor density was increased from $18.3\times10^{19}cm^{-3}$ for undoped to $27.43\times10^{20}\ cm^{-3}$ for 1.0% Zr doped sample afterword it decreased.

Photoelectrochemical Study



- Doped samples, exhibited better PEC response as compared to undoped sample and 1.0 % Zr-doped α-Fe_2O_3 was identified as best performing photoelectrode.

- This sample exhibited 754μA/cm^2 photocurrent at external bias 0.6 V/SCE and 132 μA/ cm^2 in no bias condition.
- A shift of the onset potential for photocurrent to the negative direction, from 0.6 V/SCE for undoped to -0.32 V/SCE for 1.0 % Zr doped sample

Conclusion

- Effect of Zr doping on photoelectrochemical activity of α-Fe_2O_3 has been thoroughly investigated with the supporting characterization results.
- 1.0% Zr-doped α-Fe_2O_3 sample showed significantly good photocurrent densities, which has been attributed to improved carrier density, flat band potential and peculiar morphology with optimum porosity and grain size.
- A negative shift in onset potential offers the more catalytic surface for hydrogen evolution than the undoped α-Fe_2O_3.
- It may be concluded that Zr doped nanostructured α-Fe_2O_3 thin film at optimum doping level can be efficiently used for PEC generation of hydrogen.

Thank You for Your Kind Attention