

## ***Abstract***

In the present study, a modeled framework through the use of the commercial finite element software COMSOL Multiphysics for electromagnetic analysis. Practical considerations relevant to finite element modelling are highlighted for the simulation of Mach-Zehnder–electro-optic modulator was effectively established. In particular, multi-layered Mach-Zehnder electro-optic modulator was modeled using a number of nanomaterials layers (SiO<sub>2</sub>, Si WG, and LN) and gold coplanar electrode, with respect to the Si WG layer width and thickness alteration. In this particular investigation, it was found that high Mach-Zehnder electro-optic modulator performance can be acquired using Si WG width of 2.5  $\mu\text{m}$  and thicknesses of 0.43 and 0.44  $\mu\text{m}$  alongside SiO<sub>2</sub> layer thickness of 0.5  $\mu\text{m}$ . Furthermore, the experimental work was established based on the obtained dimensions; the experimental depositions of the device layers was accomplished using Pulse Laser Deposition technique on Si-substrate and LN-substrate. Additionally, a number of characterization techniques were considered to investigate the micro-structural and optical properties of the deposited (XRD, FESEM, AFM, UV-Vis, and PL).

Specifically, the structural analysis, in particular, the XRD results, revealed that the deposited films delivered higher crystallinity using Si-substrate as compared to that deposited on the LN-substrate. The deposited film on Si-substrate demonstrated a crystallite size of 5.6 nm, while on LN-substrate was 16.6 nm. Furthermore, the morphological analysis showed that a particle size of the deposited nanomaterials could be found in the range of 30-130 nm. In the meanwhile, the thickness of

the deposited  $\text{SiO}_2$  layer and Si WG are  $\sim 400$  and  $\sim 430$  nm, respectively. AFM measurements found that the values of roughness average, RMS roughness for Si-Sub. 8.52nm ,9.84nm that is small as compared to LN-Suba. In the optical analysis, it was noticed that the energy band -gap obtained was 3.32 eV for both cases (Si-substrate and LN-substrate); while the refractive index obtained, which was used in the MZM device modeling, were 3.6101 and 3.611 for the deposited films on the Si-substrate and LN-substrate, respectively. Using the refractive index obtained using the UV-Vis technique as well as the deposited layer/s thickness from the FESEM technique, another modeling was performed concerning the fabricated MZM device. This, in turn, was compared with the pre-modeling presented before the experimental work. In detail, the fabricated MZM device delivered a considerable figure of merit ( $V\pi.L$ ) values which dwell within the range of 2.12 to 2.25 and the fabricated MZM 3 – dBe electrical bandwidth values around 50GHz at a device length of 2 cm, which can be considered as an acceptable  $V\pi.L$  value. Hereinafter, the utilization of Si-substrate indicated a better value of the  $V\pi.L$  as compared to the LN substrate, with respect to the Si WG width ( $2.5 \mu\text{m}$ ).