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Effect of Zirconium Doping on the Optical and Ferroelectric Properties of Bismuth Ferrite for Enhanced Photovoltaic Performance

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INTRODUCTION & AIM

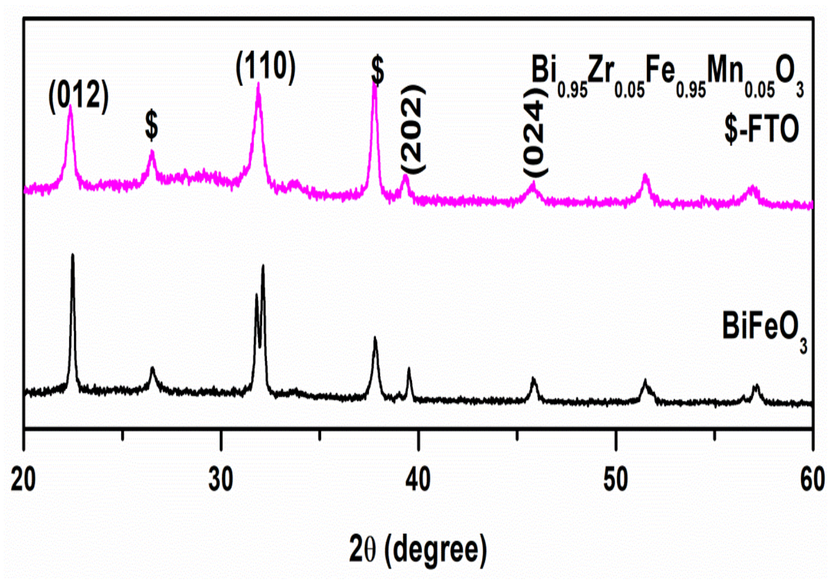
Bismuth ferrite ($BiFeO_3$, BFO) is highly regarded for its high-temperature ferroelectric and magnetic properties, making it ideal for advanced applications such as ferroelectric photovoltaic devices. This study aims to enhance BFO's performance by doping it with Zr cations. Thin films of undoped and Zr-doped BFO were prepared using the sol-gel method and spin-coated onto FTO substrates. X-ray diffraction confirmed a rhombohedral crystal structure, while UV-Vis spectroscopy indicated high transparency and a direct band gap, with the band gap narrowing upon doping, improving suitability for visible light applications. Ferroelectric measurements revealed increased saturation polarization, coercive field, and remnant polarization in the Zr-doped films. Additionally, photoconductivity tests showed reduced leakage current densities due to co-doping, indicating improved efficiency for photovoltaic devices. These findings demonstrate that Zr-doped BFO films offer significant enhancements in optical and ferroelectric properties, crucial for advancing photovoltaic technology.

METHOD

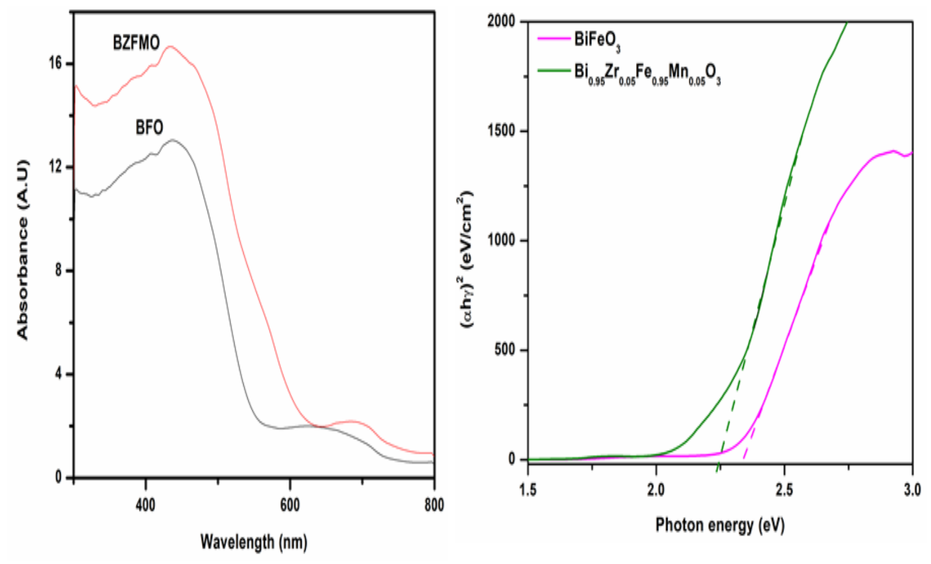
The precursor solutions of $BiFeO_3$ (BFO) and $Bi_{0.95}Zr_{0.05}Fe_{0.95}Mn_{0.05}O_3$ (BZFMO) prepared by sol-gel method were spin coated on flourine tine oxide (FTO) substrate at 3000 rpm for 30 sec. The deposited wet thin films placed on a hot plate at 150°C for 4 min were preheated at 500°C for 10 min.. By consecutive heating process, 8 layers of thin films deposited were annealed at 500°C for 1h at nitrogen (N_2) atmosphere. The crystal structure of the BFO, and BZFMO thin films were determined by X-ray diffractometer (XRD, D8 Advanced Bruker, Germany). The UV-Visible absorption studies were measured by UV-Vis spectrometer (UV-3600 Plus, Shimadzu). The ferroelectric characteristics were deduced using LC ferroelectric tester (Radiant Technology). The current density-voltage characteristics were collected from Keithley 2635B source meter under illumination with 500 W xenon lamp.

RESULTS & DISCUSSION

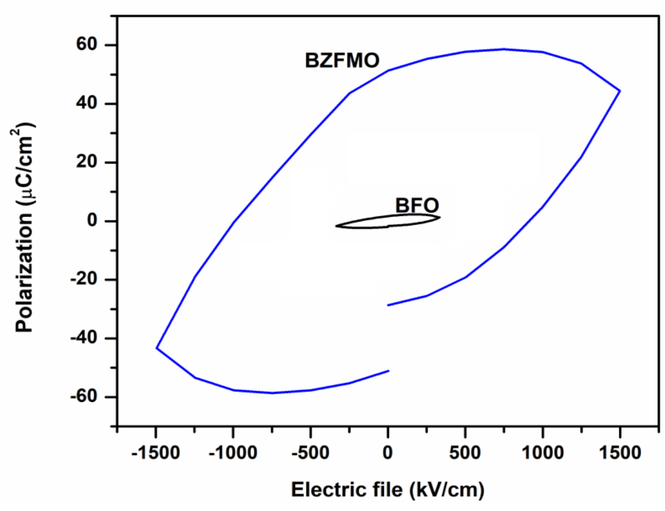
XRD pattern of BFO and BZFMO:



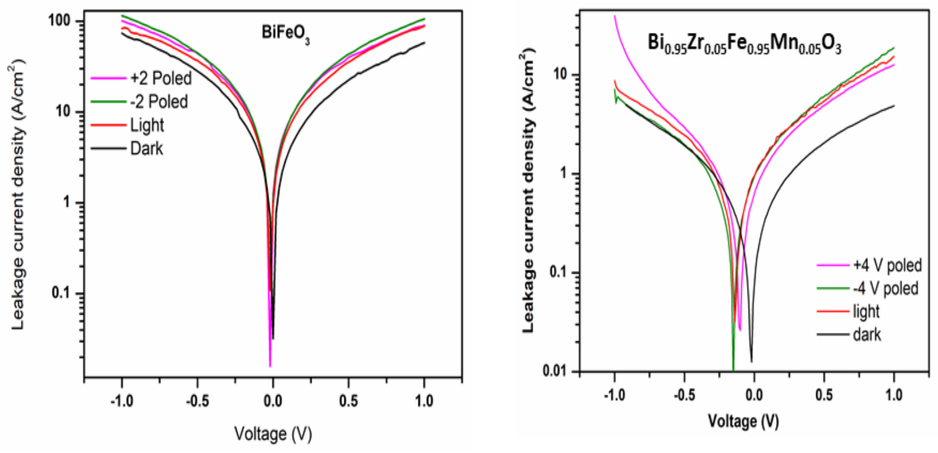
a) Absorbance spectra and (b) Tauc plot of BFO and BZFMO:



Ferroelectric response of BFO and BZFMO:



The leakage current density characteristics of BFO and BZFMO in the dark and under illumination:



CONCLUSION

In this report, we have fabricated Au/BFO/FTO and Au/BZFMO/FTO photovoltaics based on BFO and (Zr, Mn) doped BFO films by sol-gel spin coating method. Addition of Zr and Mn resulted in lattice distortion in BFO due to doping induced microstain. thereby reducing the grain size. Furthermore, enhanced absorption of UV-Vis spectra and decreased band gap was witnessed. Improved ferroelectric properties such as high remnant polarization, large saturation polarization and coercive field were observed as a consequence of (Zr, Mn) doping in BFO. Photovoltaic characterization reveals considerable reduction in the leakage current. All these favourable results indicate BZFMO as an interesting ferroelectic photovoltaic material in pursuit of high efficiency energy related device applications.

FUTURE WORK / REFERENCES

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