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Investigating the Band Gap of TiO2, Nb2O5, and AlO3 coated on Stainless Steel Electrodes used for Electrocoalescence

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INTRODUCTION & AIM

The band gap energy in semiconducting materials is crucial for electric structure and is needed for procedures like water splitting. Electrostatic coalescence is an effective method for separating water from crude oil in the petroleum industry. Electrode geometry plays a crucial role in electrocoalescence, the process of phase separation in emulsions using electric fields. It influences the distribution of the electric field applied to the emulsion, affecting coalescence efficiency. The shape and size of electrodes can also affect the electric field strength at different points in the emulsion, promoting more efficient droplet coalescence [1-2].

Electrode geometry can also influence the direction of droplet flow in the emulsion, optimizing the phase separation process. Proper geometry can minimize unwanted side effects, such as the formation of more stable emulsions or undesirable electrochemical reactions. The choice of electrode geometry can be optimized for different types of emulsions and operating conditions, improving the efficiency of the electrocoalescence process.

This study investigates the influence of electrode geometry on electrocoalescence, a process that uses electric fields to separate phases in emulsions, focusing on oil-water separation. Electrodes coated with metal oxides (TiO2, Nb2O5, and Al2O3) were designed for a static electrocoalescence cell. The optical and structural properties of the oxides were analyzed by X-ray diffraction and UV-Vis spectroscopy. The results show that the metal oxides have different band gap energies, which can be adjusted to optimize the electrocoalescence process. The indirect and direct band gap energies were determined for each oxide: TiO2 (3.18 eV and 2.96 eV), Al2O3 (4.29 eV and 3.67 eV/2.60 eV), and Nb2O5 (3.54 eV and 2.90 eV).

METHOD

The definition of the electrode geometry (Fig. 1) was performed using the FEMM 4.2 program, as a result, the electrostatic cell's optimal electric field was designed (Fig 2).

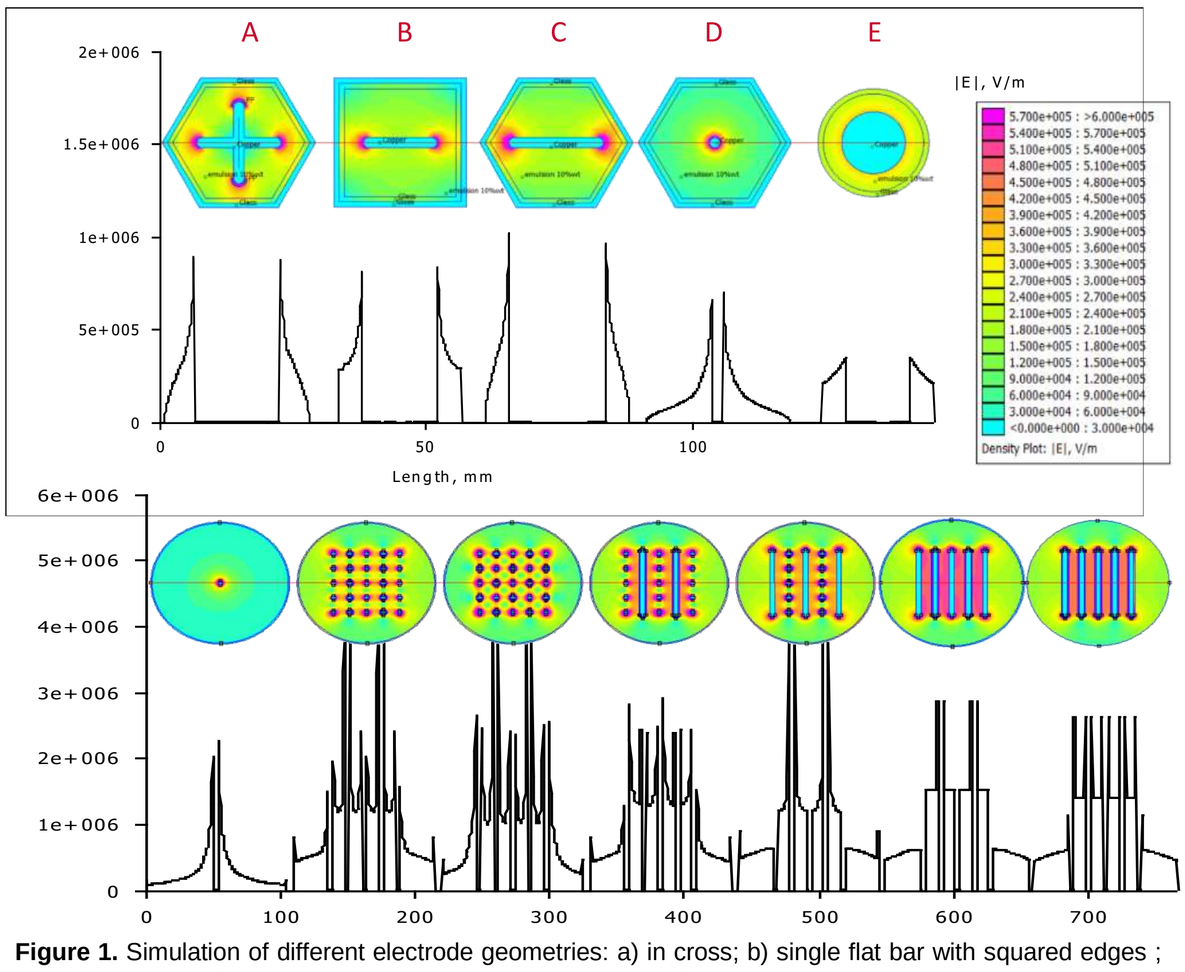

Figure 1. Simulation of different electrode geometries: a) in cross; b) single flat bar with squared edges ; c) single flat bar with hexagonal edges; d) and e) circular electrode and cell.

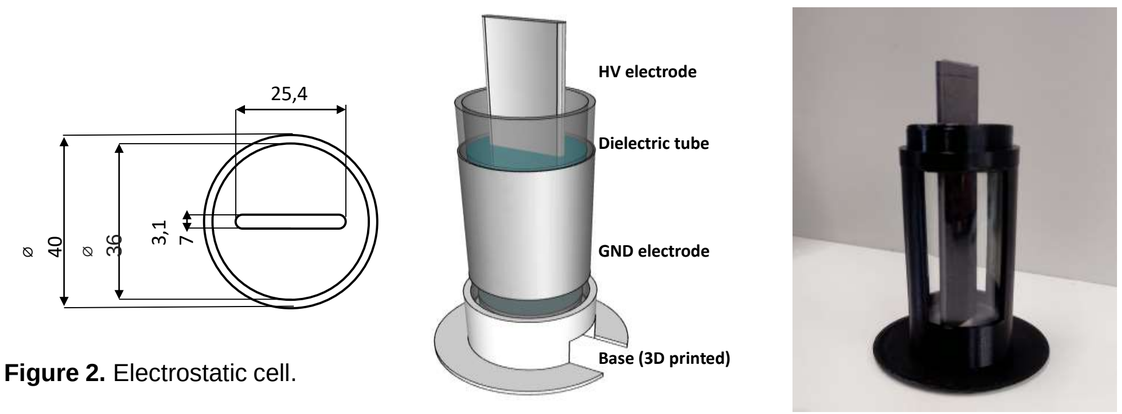

Figure 2. Electrostatic cell.

The thin films of metal oxides were deposited on stainless steel electrodes at 660 °C using N2 atmosphere using a quartz tube furnace (Lindberg/Blue M —Thermo Scientic). For characterizations, the Nb2O5, AlO3, and TiO2 in poder form were examined using Shimadzu XRD-7000 x-ray diffraction (Figure 3) and Shimadzu 2600 i UV-Vis spectrophotometry (Figure 4).

RESULTS & DISCUSSION

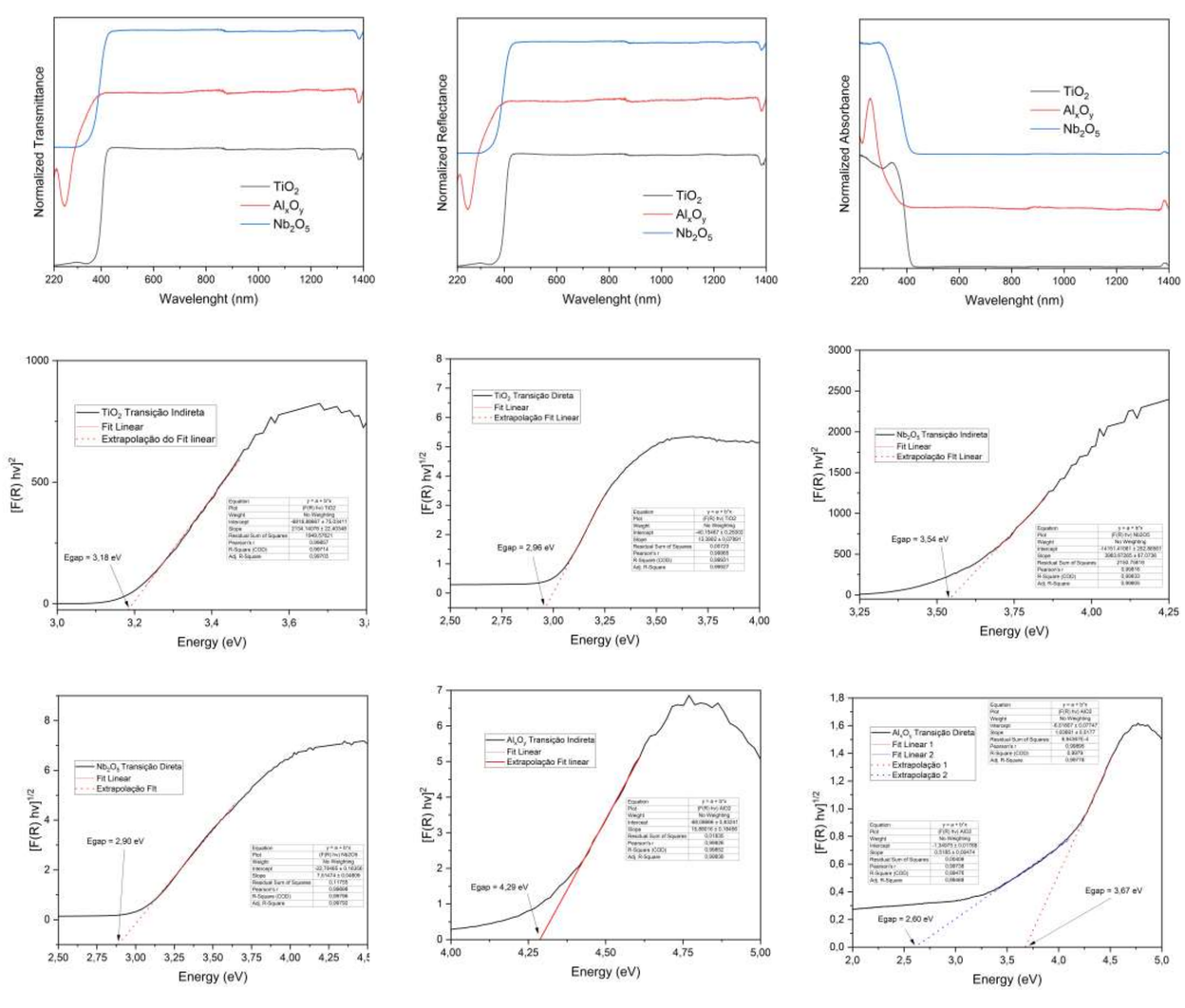

Fig. 3 X-ray powder diffractograms and band gap determination of the samples.

To determine the direct and indirect bandgap energy for the samples, the Kubelka-Munk function was applied using the reflectance spectrum. It was possible to find an indirect bandgap energy (3.18 eV, Adj. R2 = 0.99703), common for the Anatase form of TiO2 and a direct bandgap energy (2.96 eV, Adj. R2 = 0.99927), common for the Rutile form of TiO2. Both are in agreement with the literature (Anatase = 3.2 eV and Rutile = 3.0 eV). For the AlO3 sample, one indirect bandgap energy was found (4.29 eV, Adj. R2 = 0.99838), while two direct bandgap energies could be determined (3.67 eV, Adj. R2 = 0.99778; 2.60 eV, Adj. R2 = 0.99476). The Nb2O5 sample adequately presented an indirect (3.54 eV, Adj. R2 = 0.99605) and direct bandgap energy (2.90 eV, Adj. R2 = 0.99792). As for other oxides, the most suitable energy will depend on the actual polymorphic species or mixture of the sample.

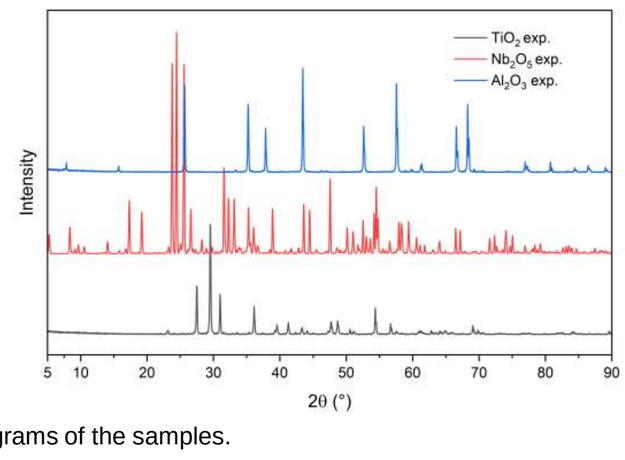

Fig. 4 UV-Vis diffractograms of the samples.

CONCLUSION

The metal oxides exhibited different band gap energies, which can be adjusted to optimize the electrocoalescence process. The indirect and direct bandgap energies were determined for each oxide: TiO2: 3.18 eV (indirect) and 2.96 eV (direct); Al2O3: 4.29 eV (indirect) and 3.67 eV/2.60 eV (direct); Nb2O5: 3.54 eV (indirect) and 2.90 eV (direct). The results suggest that the choice of metal oxide and electrode geometry can be optimized to improve oil-water separation efficiency. Determining the bandgap energies of metal oxides is essential for understanding and optimizing the electrocoalescence process.

FUTURE WORK / REFERENCES

[1]. KHAN, M.M. Chapter 6 - Common characterization techniques for photocatalytic materials. *Theoretical Concepts of Photocatalysis*, 2023, Pages 115-154.
[2]. WU, Y.; LI, B.; JU, M.; XIANG, W.; SUN, Z.; WANG, H.; YU, K.; WANG, Z.; WANG, J. Nanoparticle-laden droplet-liquid film electrocoalescence behaviors: A molecular dynamics simulation. *Journal of Molecular Liquids,* 400, 15, 2024, 124553.