

Modeling Piezoelectric and Flexoelectric Response of ZnO Nanopillars under Cavitation-Induced Bending in Water

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Zinc oxide (ZnO) is a widely studied, non-centrosymmetric semiconductor known for its strong electromechanical coupling. Due to these properties, ZnO has attracted significant attention for energy-harvesting technologies, where bending, vibration, or pressure variations can be converted into usable electrical energy. In this work, we present a theoretical study of ZnO nanostructures under cavitation-induced bending in water using COMSOL Multiphysics. The model simulates the electric potential generated by piezo- and flexoelectric effects and provides a framework for its application to water-splitting reactions driven by ultrasound or pressure fronts. The obtained results show that ultrasonic heterogeneous cavitation ($\sim 40\text{kHz}$ at an effective power of 0.1- 0.2 W) can generate local deformation via strain fields (flexoelectricity) and compression (piezoelectricity). The magnitude of these polarisations depends directly on the size and morphology of the ZnO nanostructures. We identified that pillar-like structures with micrometre lengths and nanometer diameters are optimal for strain-driven catalysis.[1] Under working conditions, the potential exceeds 0.1V for both piezo- and flexoelectric polarisations. The presented approach contributes to the development of cavitation-driven electromechanical systems for aiding water-splitting reactions and related electrochemical applications.

References:

[1] M. Kołodziej, N. Ojha, M. Budziałowski, K. Załęski, I. Fina, Y. K. Mishra, K. K. Pant and E. Coy, *Small* 20 (2024) 2406726

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