Project title
Organic Solar Cells Fabricated Under Ultrasonic Capacitance Spectroscopy Supported by Machine Learning

Principal Investigator
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1. Current Status of the Problem

The growing global demand for renewable energy sources continues to drive the active development of photovoltaics, which remains one of the most promising approaches to achieving sustainable and clean energy production. In this context, organic solar cells (OSCs) are receiving increasing attention as representatives of a new generation of phototransducers that combine low manufacturing cost with the potential use of environmentally friendly materials. Despite these advantages, OSCs face several significant limitations, including relatively low power conversion efficiency and pronounced susceptibility to degradation. Both challenges are largely influenced by the state of the defective subsystem of the material.One of the most effective strategies for improving the stability and performance of OSCs is the controlled modification of the fabrication process to achieve targeted defect engineering. This approach enables deliberate control over the structure and electronic properties of the resulting nanostructures.

One of the approaches to modifying the defective subsystem is the excitation of elastic waves. Research shows that acoustic waves in non-piezoelectric materials can induce the redistribution of impurities and the rearrangement of point defects. This effect occurs selectively in regions with disrupted periodicity and can be observed at low temperatures. Ultrasonic treatment, used as an auxiliary factor during technological processes such as ion implantation, is particularly effective when the system is in a nonequilibrium state. Even low-intensity acoustic waves are able to cause significant changes in material properties.

At the same time, the use of ultrasound in solar cell manufacturing remains limited. The most common applications include ultrasonic cleaning, ultrasonic surface texturing, ultrasonic bonding of metallic contacts, and the formation of material layers through sonochemical reactions or ultrasonic spray coating. However, the number of studies in this area is still small, and the use of ultrasound as an auxiliary factor during standard technological operations has received very little attention.

The presence of defects in materials requires methods that enable detailed characterization. Capacitance spectroscopy provides access to information about the defect energy spectrum, although the analysis of such spectra is complex and its sensitivity to specific defects is limited. Modern machine learning (ML) methods, which are already used to enhance various experimental techniques, for example to separate the contribution of low-concentration radiation-induced defects in Raman spectra, can improve the accuracy and speed of interpreting capacitance spectroscopy data.

2. The project novelty

The first part of the project focuses on experimentally identifying the regularities associated with the effects of ultrasound loading used as an auxiliary and corrective factor during the OSCs fabrication of organic solar cells, specifically during technological steps such as spin coating, isothermal dwelling at room temperature, and annealing. The aim of these studies is to determine the ultrasonic modes that can induce a rearrangement of the defect structure and consequently increase photoelectric conversion efficiency and suppress degradation. The second part of the project focuses on developing machine learning models that analyze the frequency dependence of the capacitance of photovoltaic structures and enable the rapid detection of weak signals associated with various defects. The objectives of both parts of the project remain unresolved, although they are critically important for the advancement of the field.

3. Research Methodology

The experimental part of the project involves the fabrication of Si/PEDOT:PSS structures using a standard technological sequence that includes the following steps: i) cleaning the Si surface in an HF solution; ii) spin coating of the PEDOT:PSS solution layer; iii) room temperature relaxation hold; iv) annealing of the samples at elevated temperature; v) vacuum deposition of metal contacts. During steps two through four, acoustic excitation in the structures is planned and will serve as an auxiliary factor that influences the defect subsystem. The parameters to be varied include the type of excited waves such as longitudinal and radial modes, their frequency within the range of 0.5 to 5 MHz, and their intensity of up to 1 W/cm^2. To ensure comprehensive characterization of the fabricated structures, to identify changes in their parameters induced by ultrasound loading, and to clarify the mechanisms of acoustically stimulated modification, the following methods will be applied: current–voltage and capacitance–voltage measurements, determination of the spectral dependence of quantum efficiency, and capacitance and impedance spectroscopies.

The development of the ML models includes the simulation of capacitance spectra that correspond to different defect compositions in barrier structures in order to create a training dataset. It also includes the tuning of regression models that employ algorithms such as neural networks, random forest, gradient boosting, and support vector regression. Model testing is planned using both synthetic and experimental data.

4. Justification of the Participant's Capability to Implement the Project

O.Ya. Olikh has 30 years of scientific experience. He is the author of over 110 publications, including 20 articles in Q1 and Q2 journals. He has extensive expertise in studying the effects of ultrasound on the properties of semiconductor structures, primarily silicon-based, conducting electrophysical investigations, and applying machine learning methods for defect characterization, as evidenced by his publications.

5. Expected Outcomes of Project Implementation

The expected scientific outputs of the project include:

1) elucidation of the physical mechanisms and regularities by which elastic waves in the ultrasonic range influence the defect system of Si/PEDOT:PSS structures;
2) assessment of the potential for targeted control of the characteristics of organic solar cells through the application of ultrasound loading during the OSC fabrication process;
3) development of machine learning models aimed at determining defect parameters from capacitance spectra;
4) preparation of at least one paper in a Q1 or Q2 journal.
5) preparation of at least two presentations for international conferences.