Ultrasound Engineering as Active Tool to Drive Electronic Properties of Silicon - Polymer Interface

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Ultrasound (US) was extensively utilized as an active tool at various stages of semiconductor device manufacturing. For instance, its potential in industrial applications has been demonstrated by exciting acoustic waves in silicon targets during ion implantation [1]. One notable advantage of this approach for modifying semiconductor systems is its broad versatility, which arises from the ability to adjust the type of oscillations, frequency, and intensity of the ultrasound, as well as its sustainable and environmentally friendly nature. As a result, ultrasound is being increasingly applied in fabricating thin film photovoltaic systems. For example, the effectiveness of ultrasonically generated spray techniques has been established [2], along with the use of ultrasound during forming contacts [3]. Furthermore, enhancements in photovoltaic properties have been observed when acoustic vibrations are applied to the substrate during the spray deposition of polymer layers [4]. Our study aimed to explore the potential of using ultrasound to control the interface properties of silicon-polymer systems fabricated via spin coating. This focus was motivated by two key factors: first, these systems are among the most promising candidates for next-generation photovoltaic converters, and second, their properties are predominantly influenced by the interface.

The n-Si/PEDOT:PSS structures were fabricated as follows. A PEDOT:PSS layer was deposited on a cleaned silicon substrate by spin coating for 60 seconds. The structures were kept at room temperature for 20 minutes, then baked at 140 °C for 15 minutes. For some samples, an additional step was used: ultrasound treatment (UST) during isothermal holding at room temperature. Two types of acoustic waves were employed: longitudinal (UST-L, 2.5 MHz) and radial (UST-R, 500 kHz). Polymer layers of different thicknesses, fabricated using two spin-coating speeds (3000 and 5000 rpm), were also studied.

The electronic properties of the structures were determined via capacitance-frequency and capacitance-voltage measurements. Frequency-dependent data were collected from 100 Hz to 1 MHz at 0 and 0.4 V biases, enabling estimation of the density of states (DOS) near the interface. Without ultrasound, measurements at zero bias showed a single DOS peak ~300 meV above the valence band edge, likely due to Pb centers (dangling bonds). Under forward bias, an additional energy level at E_v+0.38 eV appeared, more prominent in thinner PEDOT:PSS layers. UST modified the DOS depending on wave type and polymer thickness (see Fig. 1): UST-R amplified the deep-level peak, while UST-L suppressed it. Capacitance-voltage measurements at 10 kHz, 100 kHz, and 1 MHz enabled the estimation of the built-in potential (V_b) from the reverse branch and the effective hole injection voltage (V_p) from the forward branch. At 10 kHz, V_b was 0.65 V, matching the work function difference between Si and PEDOT:PSS. At higher frequencies, V_b increased, indicating an additional dielectric layer, whose effect was reduced by UST. UST-L also decreased V_p.

The obtained results show that ultrasound effectively controls the electronic properties of organic heterostructures, with different wave types enabling tailored modifications.

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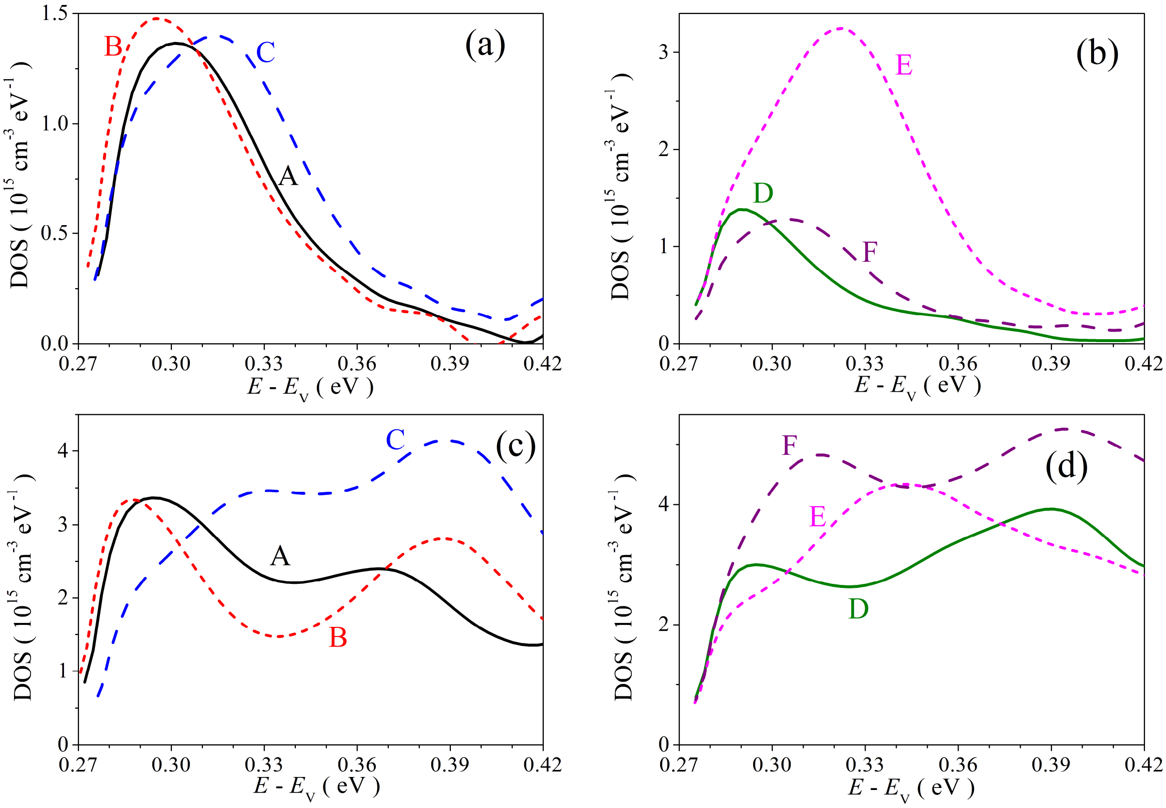

Figure 1: The density of states profiles for silicon / PEDOT:PSS structures manufactured with (curves B, C, E, and F) and without ultrasound loading (A and D). Type of ultrasound vibration: longitudinal (B, E), radial (C, F). The velocity of spin coating, rpm: 3000 (A, B, C, panels a and c), 5000 (D, E, F, panels b and d). The bias voltage, V: 0 (a, b), 0.4 (c, d).

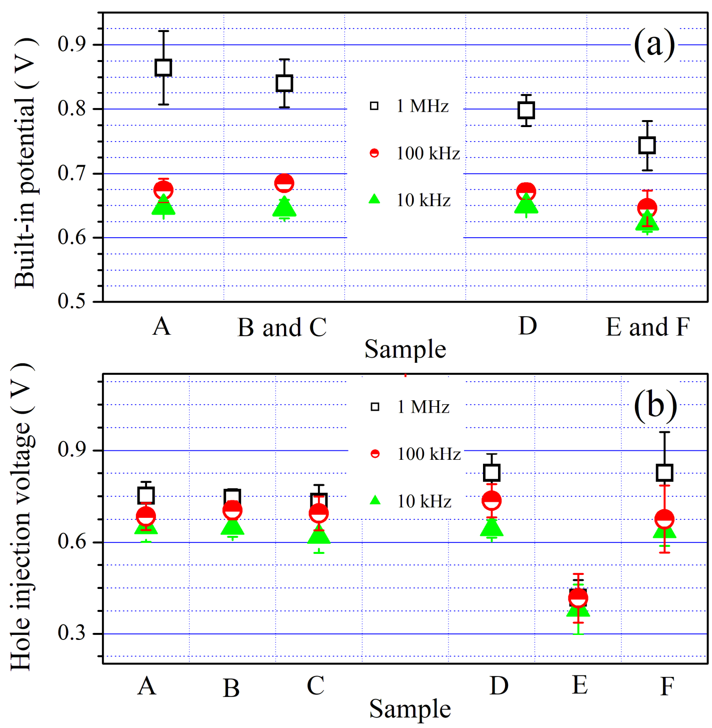

Figure 2: Built-in potential (a) and voltage of effective hole injection (b) for silicon / PEDOT:PSS structures manufactured with and without ultrasonic loading. The sample designation coincides with Fig. 1.