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碩士論文

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Master's Thesis

結合電性量測與等效電路模型於低溫與低頻率之鈣鈦礦太陽

能電池深缺陷分析

Deep Defect Analysis of Perovskite Solar Cells under Low Temperature
and Low Frequency via Electrical Measurements and Equivalent Circuit

Modeling

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中文摘要

鈣鈦礦太陽能電池（Perovskite Solar Cells, PSCs）因其高光吸收係數等優點受到廣泛關注。然而，材料內部形成的缺陷仍限制元件的穩定性與性能。因此發展一套能有效探測與分析缺陷性質之方法，對於未來太陽能電池優化具有相當關鍵的意義。

本研究針對同一個反式 P-I-N 鈣鈦礦太陽能電池，結合多項電性量測技術與等效電路分析模型，系統性的探討鈣鈦礦太陽能電池於低溫與低頻環境下之缺陷特性。量測方法包含：DLCP (Drive-Level Capacitance Profiling)、CV (Capacitance-Voltage)、TAS (Thermal Admittance Spectroscopy)、DLTS (Deep Level Transient Spectroscopy)，並利用 IS (Impedance Spectroscopy) 結果建立等效電路模型。所有實驗針對同一元件進行，並於實驗前後分別進行照光之 IV 測試以確認樣品穩定性。光電轉換效率由原來的 18.62% 降為 18.20%，表示樣品維持良好穩定性。

TAS 量測透過變溫條件與阿瑞尼斯圖 (Arrhenius plot) 擬合，得到缺陷活化能為 45.7 meV，淺層陷阱密度約為 $8.84 \times 10^{14} \text{ cm}^{-3}$ 。DLTS 成功分離出電子、電洞陷阱，其中電子、電洞陷阱能量深度為 511.4 meV、660.4 meV；陷阱密度約為 $5.86 \times 10^{13} \text{ cm}^{-3}$ 、 $5.35 \times 10^{13} \text{ cm}^{-3}$ 。CV 分析求得內建電壓值約為 1.076 V，摻雜濃度約為 $2.03 \times 10^{16} \text{ cm}^{-3}$ 。透過 DLCP 與 CV 結果比較，可推得樣品缺陷密度於空間中的分布與界面效應。最後透過利用等效電路模擬阻抗圖譜，發現樣品於低頻區間出現明顯電荷累積與界面極化，對應之界面電容約為 45.7 nF。

綜上所述，本研究建立一套以單一樣品為對象的缺陷量測流程，涵蓋空間、能階深度與頻率響應等。本研究結果對於鈣鈦礦太陽能電池之缺陷診斷具有高度參考價值。

關鍵字：鈣鈦礦太陽能電池、缺陷密度、光電轉換效率、TAS、CV、DLCP、DLTS、阻抗分析、電路模擬

Abstract

Perovskite solar cells (PSCs) have attracted extensive attention due to their advantages such as high optical absorption coefficients. However, defects formed within the material still significantly limit device stability and performance. Therefore, developing effective methods to probe and analyze defect properties is crucial for the future optimization of perovskite solar cells.

In this study, a single inverted P-I-N structured perovskite solar cell was investigated by integrating multiple electrical characterization techniques with equivalent circuit modeling to systematically explore defect characteristics under low-temperature and low-frequency conditions. The measurement techniques employed include capacitance–voltage (CV), drive-level capacitance profiling (DLCP), thermal admittance spectroscopy (TAS), deep-level transient spectroscopy (DLTS), and impedance spectroscopy (IS), from which equivalent circuit models were constructed. All measurements were performed on the same device, and illuminated current–voltage (I–V) measurements were conducted before and after the experiments to verify device stability. The power conversion efficiency decreased slightly from 18.62% to 18.20%, indicating that the device maintained good stability throughout repeated measurements.

TAS measurements combined with temperature-dependent analysis and Arrhenius fitting revealed a shallow defect level with an activation energy of 45.7 meV and a trap density of approximately $8.84 \times 10^{14} \text{ cm}^{-3}$. DLTS measurements successfully distinguished electron and hole traps, with energy depths of 511.4 meV and 660.4 meV and corresponding trap densities of $5.86 \times 10^{13} \text{ cm}^{-3}$ and $5.35 \times 10^{13} \text{ cm}^{-3}$, respectively. CV analysis yielded a built-in potential of approximately 1.076 V and an estimated doping concentration of $2.03 \times 10^{16} \text{ cm}^{-3}$. By comparing DLCP and CV results, the spatial distribution of defect density and interfacial effects within the

device were further inferred. Finally, impedance spectroscopy combined with equivalent circuit modeling revealed pronounced charge accumulation and interfacial polarization in the low-frequency region, with an interfacial capacitance of approximately 45.7 nF.

In summary, this work establishes a defect characterization framework based on a single device, covering spatial distribution, energy depth, and frequency response of defects. The results provide valuable insights for defect diagnosis in perovskite solar cells.

Keywords: Perovskite Solar Cells, Defect Density, Power Conversion Efficiency, TAS, CV, DLCP, DLTS, Impedance Analysis, Circuit Simulation