Modelling and Loss Analysis of Meso-structured Perovskite Solar Cells

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Introduction:

The pursuit of organic-inorganic perovskite solar cells (PSC) has been significantly advanced because of the promising high-efficiency potential of the perovskite materials. The latest certified best efficiency is 22.1%. In addition to the advancement in experimental studies, the modelling and numerical simulation of PSC are crucial, as it aids in elucidating the device physics, unveiling its intrinsic material properties and predicting the device performance. In this work, we

- ❑ Derive a mathematical model for meso-structured perovskite solar cells and calibrate it towards intensity dependent current voltage (IV) measurements.
- ❑ Identify the main recombination loss channels. Quantify the interface recombination between the mesoporous perovskite and the mesoporous titanium dioxide.

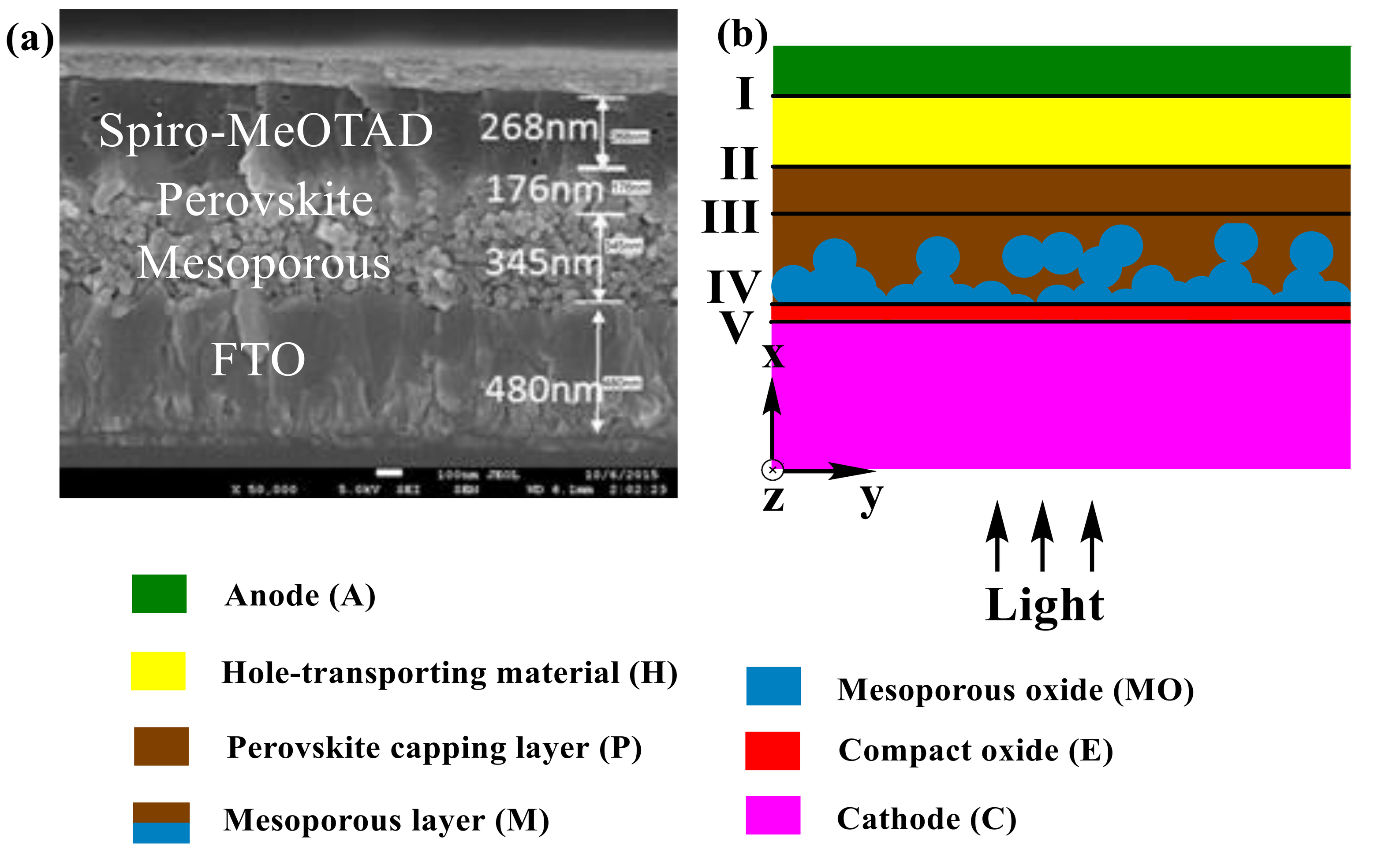

Fig. 1: (a) A SEM image of the fabricated meso-structured PSC; (b) Schematics of the meso-structured PSC with six layers and five interfaces.

Semiconductor physics

- ❑ Use Transport of Diluted Species interface to compute the concentration of electrons and holes inside the solar cell:

$$\nabla \cdot \mathbf{J}_h = G - R,\quad \mathbf{J}_h = -D_h \nabla C_h - C_h \mu_h \nabla \psi$$
$$\nabla \cdot \mathbf{J}_e = G - R,\quad \mathbf{J}_e = -D_e \nabla C_e + C_e \mu_e \nabla \psi$$

coupled with Poisson's Equation interface to model the electric potential within the cell

$$\nabla \cdot (\varepsilon \nabla \psi) = e(C_e - C_h)$$

where $\mathbf{J}_h/\mathbf{J}_e$: flux of hole/electron; G/R: generation and recombination rate of electron and holes; C_h/C_e: hole/electron concentration; D_h/D_e: diffusion coefficients; μ_h/μ_e: motilities; ψ: electric potential; ε: permittivity; e: elemental charge.

- ❑ Enforce interface boundary conditions for electric potential, electric field, electron/hole flux, electron/hole concentration.

Optics: transfer matrix method

- ❑ G is expressed as $\frac{\theta}{h\nu}Q$, with Q being the time average of the energy dissipated per second at normal incidence:

$$Q = 2\pi\nu\varepsilon_0\eta_{eff}\kappa_{eff}|E_{eff}|$$

where η_{eff} and κ_{eff} are defined by volume averaging theory

$$\eta_{eff} = \frac{1}{2}\left(X + \sqrt{X^2 + Y^2}\right),\qquad \kappa_{eff} = \frac{1}{2}\left(-X + \sqrt{X^2 + Y^2}\right),$$

$$X = \phi\left[(\eta^P)^2 - (\kappa^P)^2\right] + (1-\phi)\left[(\eta^E)^2 - (\kappa^E)^2\right],$$

$$Y = 2\phi\eta^P\kappa^P + 2(1-\phi)\eta^E\kappa^E.$$

- ❑ η and κ are refractive index and extinction coefficients obtained from ellipsometric measurements, ϕ is porosity.
- ❑ Perform cubic spline interpolation after importing G profile inside COMSOL.

Calibration and validation

- ❑ Calibration of 5 unknown recombination parameters in least-squares sense in LiveLink for MATLAB by finding

$$\Phi = \left(B^P_{rad}, A^P_{Aug}, \tau^P_{SRH}, D^M_{eff}, S_{eff}\right)$$

that best fit the expression

$$\min\left\|\mathbf{I}(\boldsymbol{\Phi}, \boldsymbol{V}_{ap}) - \mathbf{I}^{measure}(\boldsymbol{V}_{ap})\right\|^2$$

at illumination intensities of 0.3 sun as the training set and validated at 0.5 and 1 sun as the test sets

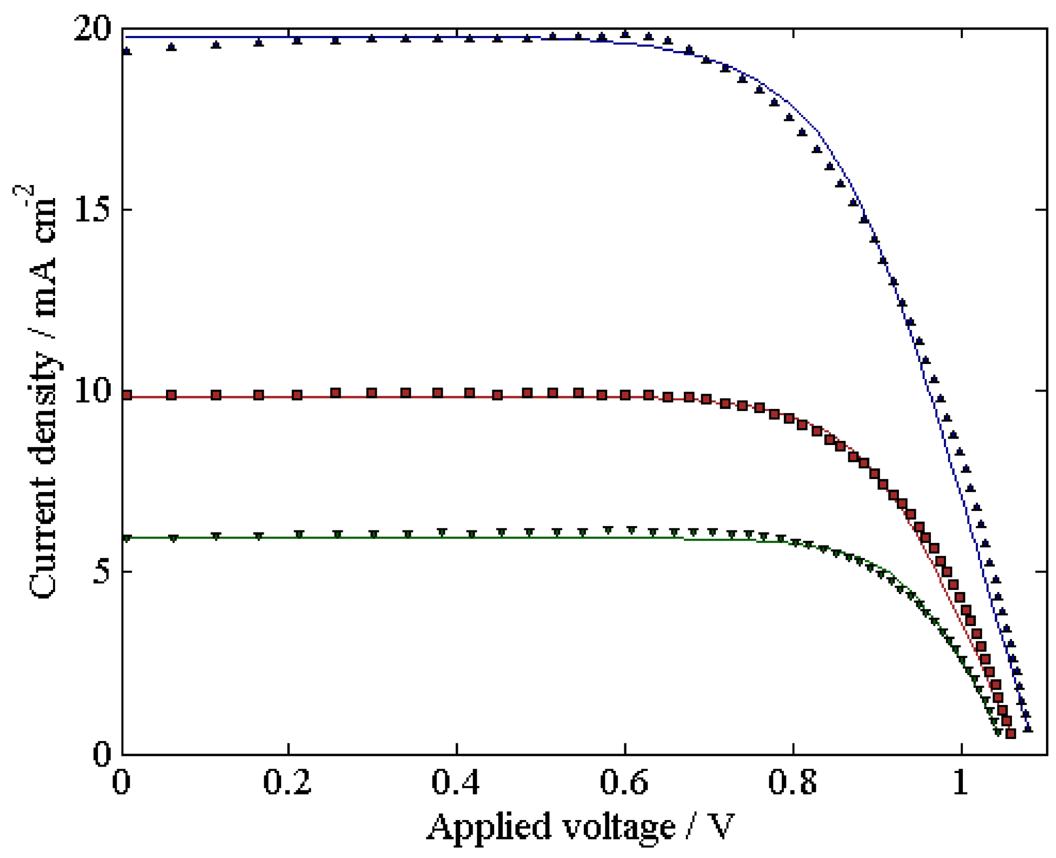

Fig. 2: Predicted (lines) and measured (symbols) current-voltage curves for meso-structured PSC under an AM 1.5 solar illumination.

Result: loss analysis

- ❑ Radiative recombination dominates within the perovskite capping layer, whereas the dominant recombination from the mesoporous layer occurs at the perovskite/TiO_2 interface.

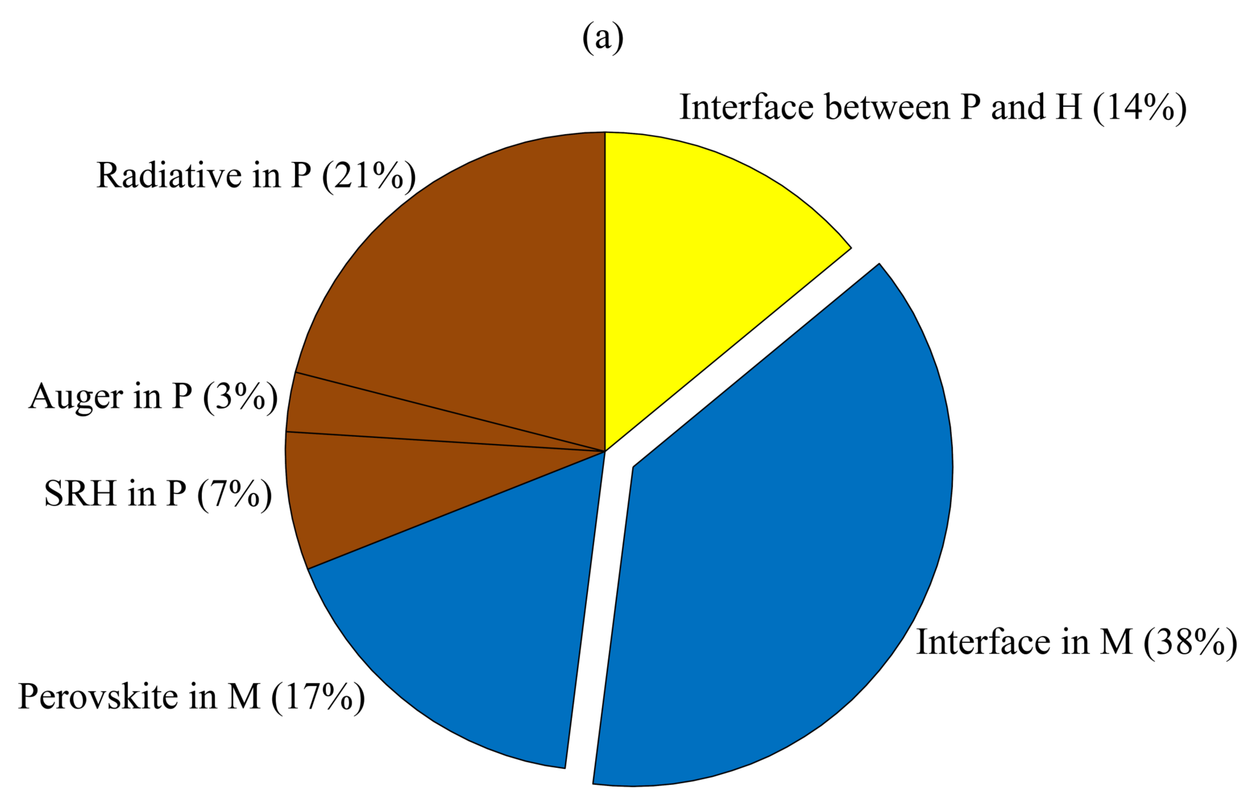

Fig. 3: Percentage contribution of various recombination loss channels under open-circuit condition.

Outlook

- ❑ With the developed device model, the different device performance of a planar-structured PSC and a meso-structured PSC shall be compared.
- ❑ A three dimensional explicit modelling of the mesoporous layer for validation of the 1D effective-medium approach shall be undertaken.

Reference: H. Xue, K. Fu, L. H. Wong, E. Birgersson, R. Stangl, J. Appl. Phys. 122, 083105 (2017)

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