Simple Determination of Optical Constants of Organic Blends

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Introduction

- Organic solar cells (OSCs) are in great demand recently due to their low-cost fabrication, non-toxicity, and compatibility with roll-to-roll large-scale processing and semitransparency.
- For OSCs, as well as other solar cells, the optical constants (refractive index,n, and extinction coefficient) can be used in preliminary analysis of maximum achievable photocurrent.
- In the OSCs, the blend of a donor and an acceptor material is used in the active layer of OSC.
- Thus, for analysis of OSCs, the determination of optical constants of organic blends is necessary.This determination by sample fabrication and ellipsometry processes is money and time consuming.
- In this study, we introduce a method for calculation of optical constants of the blends made out of any concentration ratio of donor and acceptor organic materials. This process removes the need for ellipsometry and sample fabrication steps for different blend ratios.
- The method is based on the the principle of mixtures, in which optical constants of individual materials are scaled according to compositions.

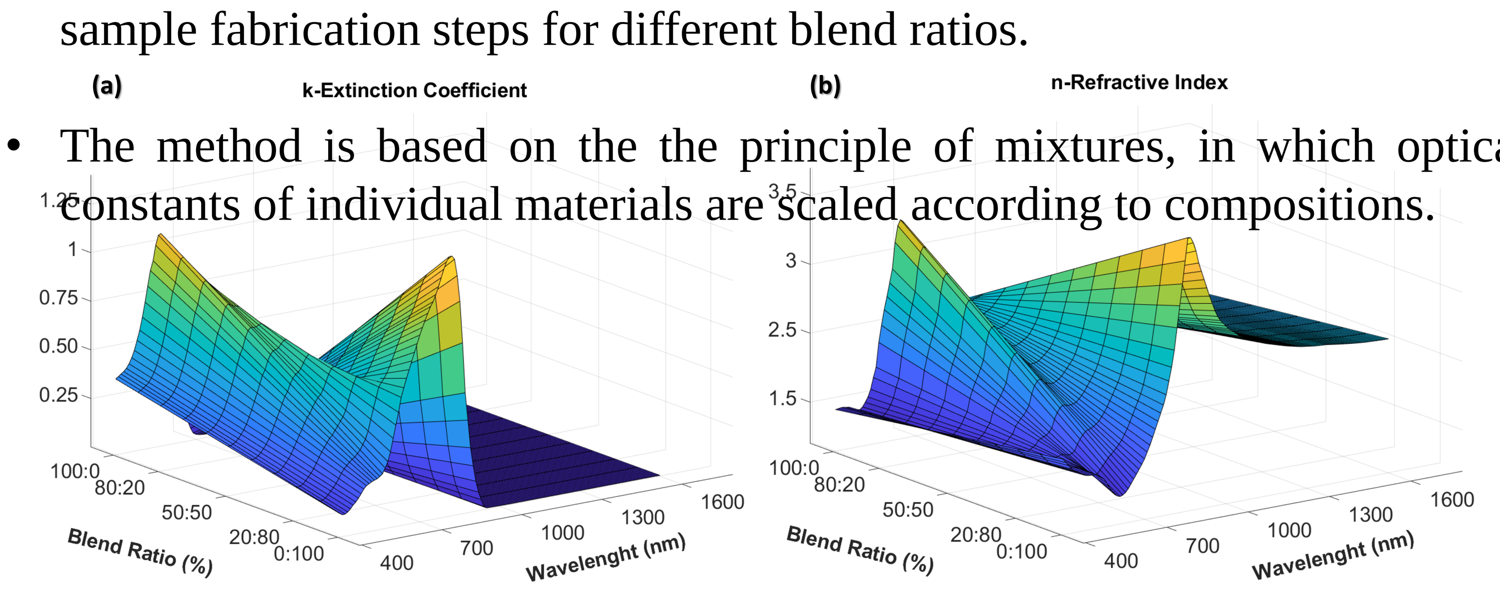

Figure 1: Calculated Optical Coefficients (n&k) of PM6:Y6 Blend with Varying Ratios

Methodology

- The transmission data of donor and acceptor materials are obtained experimentally, via transmission spectrometry.
- Transmission data is used to obtain the refractive index (n) and extinction coefficients (k) of blend components with the method introduced by Kerremans et al. [1], which bases on mainly transmission fitting in the Cauchy regime, Transfer Matrix Method (TMM), and Kramers Kronig relations. Figure 2 depicts the accuracy level of this method.

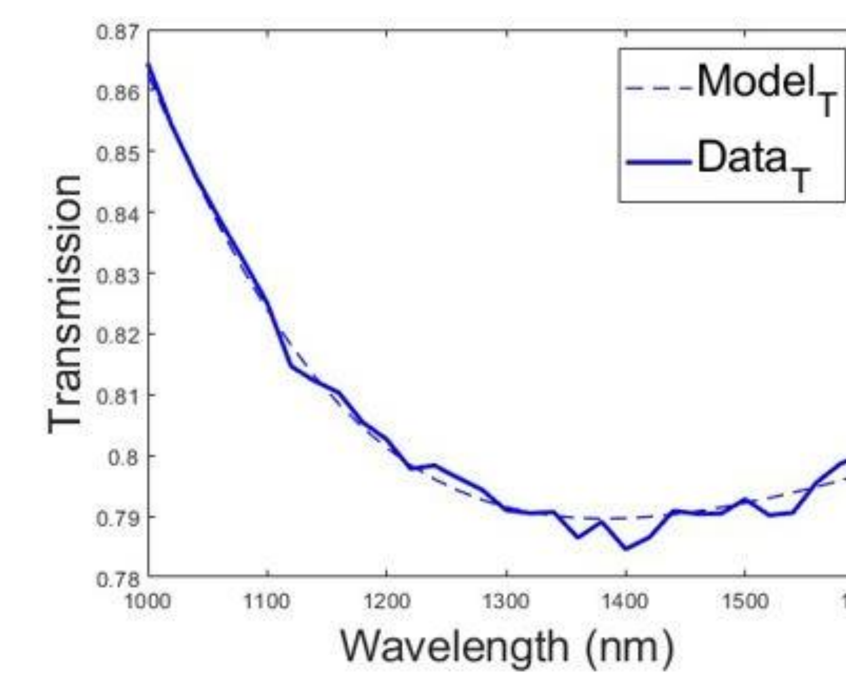

Figure 2: Experimentally measured (solid) and fitted (dashed) transmission of a blend PM6:Y6.

- While the n/k values are the inputs of any optical optimization process on thickness, introduction of the of the calculated n/k values for varying cases makes the blend ratio also an optimization parameter.
- After complete implementation of this new method to an optimization system, best blend ratio and thickness become a collective result of only one process, as described in Figure 3.
- This process contains TMM and AVT evaluation analysis with optimum thickness and blend ratio fitting, all constructed via MATLAB.

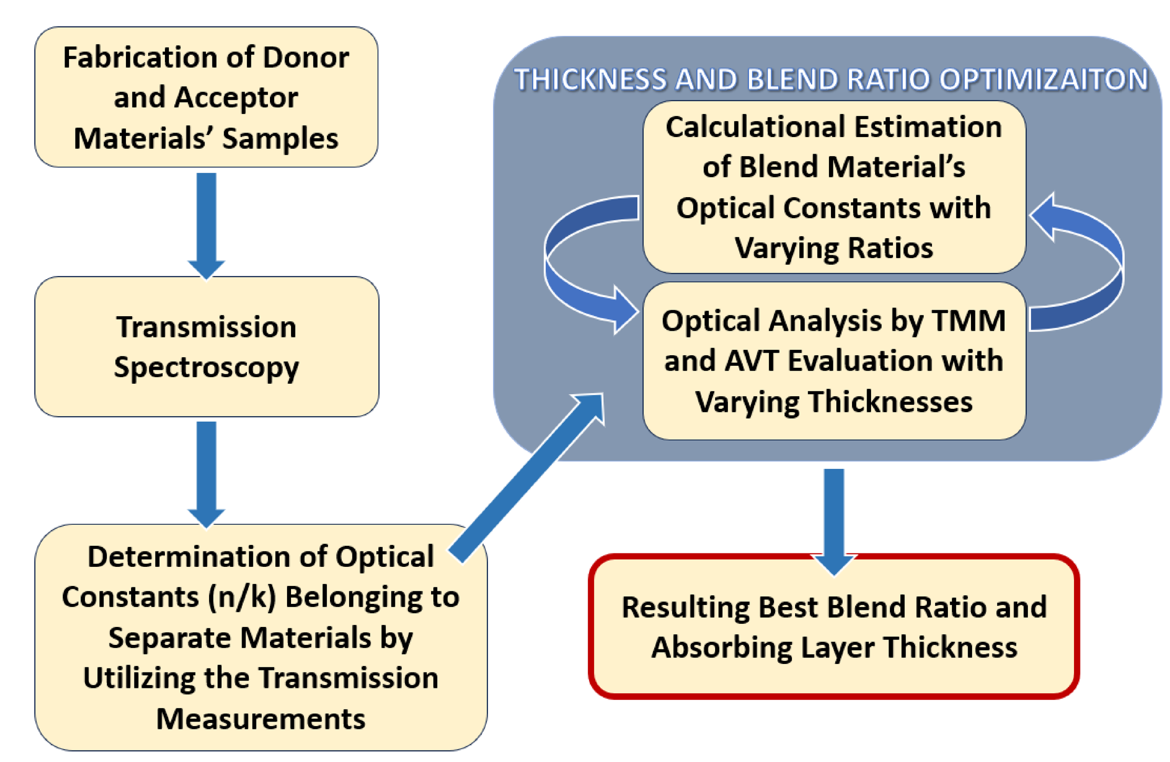

Figure 3: Workflow of the Absorber Optimization Methodology

Results

- Calculated optical constants of varying "unproduced" blends are compared with the optical constants that are obtained by the Kerremans' method mentioned in [1] based on the measured transmission spectrum of synthesized blends.
- As seen in Figure 4, rule of mixture provides satisfying results for different cases.
- By the help of quick estimation of optical constants of the blend material that are used for OSC's active layers, OSC optimizations are performed for highest short circuit current (J_{sc}) and average visible transmission (AVT) as fundamental demonstrations.

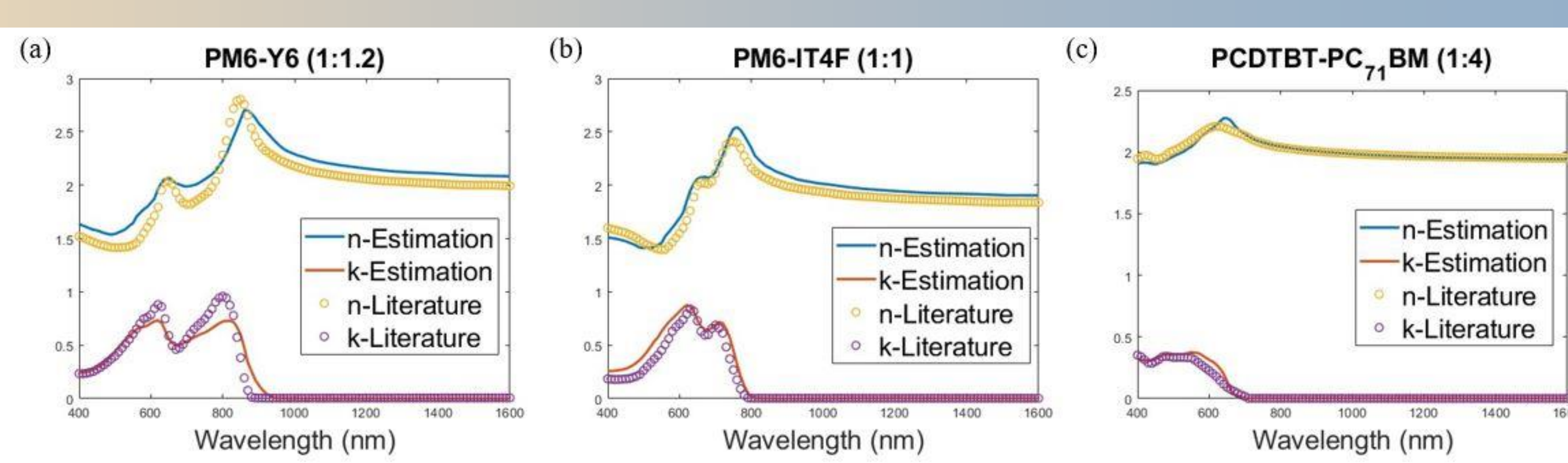

Figure 4: Determined n/k of (a)PM6:Y6, (b)PM6:IT4F and (c)PCTBT-PC$_{71}$BM by Kerremans' method from [1] and by proposed method

- According to the blend ratio of the materials and the thickness of the active layer, Figure 5 is created. For PM6:Y6, highest J_{sc} is obtained as 22.72 mA/cm^2 for 2:3 ratio and 330 nm thickness. For PM6:IT4F, highest J_{sc} is obtained as 23.46 mA/cm^2 for 1:1 ratio and 400 nm thickness. As given in (a) and (d), respectively.

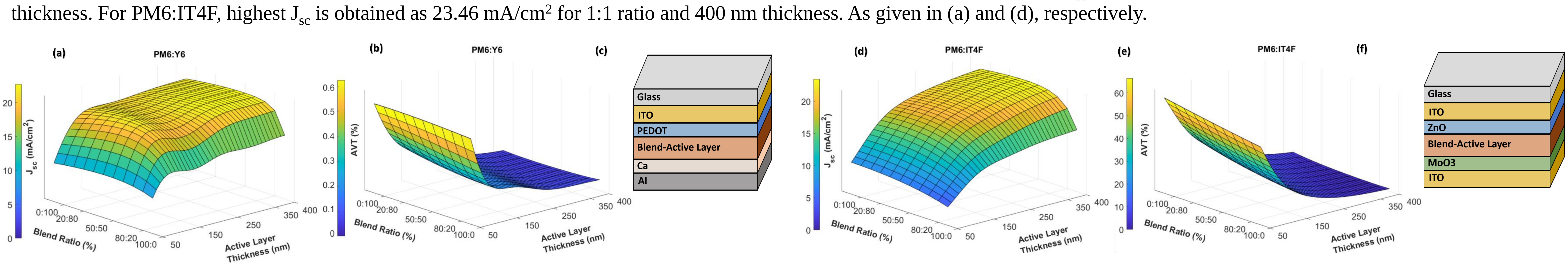

Figure 5: OCS properties according to the blend ratios and the active layer thicknesses, (a)Jsc of PM6:Y6 (b)AVT of PM6:Y6 (c)Jsc of PM6:IT4F (d)AVT of PM6:IT4F

- In (b) and (e), AVT percentages are provided with the same coordinates for suitability of comparison with J_{sc}.
- Different device structures are used for AVT improvement. The highest values of AVT are 0.63% and 66.48% for the structures in (c) and (f), respectively.
- A reasonable approach for a semitransparent OSC might be targeting the highest J_{sc} with ~40% threshold in AVT, resulting 11.88 mA/cm^2 and 39.53% AVT for structure in (f).

Conclusion

- The core concept is the ability to obtain the n/k values of blends with any blend ratio. The scope of this study is a valuable step for further studies on improvements of organic solar cells.
- The structure of the layers apart from the active layer contributes greatly on the level of AVT and short circuit current. The computer-based calculations provided can work with various layer materials and structures, with AVT and Jsc results of that structure given as outcome. Thus, an incomparably great number of different structures could be assessed using this tool, compared to fabrication of blends and layer structures one-by-one.
- Hence, the study provides a relatively short, effortless and cost-saving approach on the optical constant analysis of blends, with the aim of ease on solar cell optimization.

References

[1] Kerremans, R., Kaiser, C., Li, W., Zarrabi, N., Meredith, P., Armin, A., The Optical Constants of Solution-Processed Semiconductors—New Challenges with Perovskites and Non-Fullerene Acceptors. Adv. Optical Mater. 2020, 8, 2000319. https://doi.org/10.1002/adom.202000319

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