S-shape properties in the J-V curves of bilayer heterojunction organic solar cells

Research students: Jingchuan Wang

A. Motivation

"S-shape" effect frequently appears in the J-V curves, which reduces the fill factor (FF) significantly, especially in tandem structures due to incomplete recombination of charge accumulation.

(i) S-shape effect on fill factor (FF)

\[ \eta = \frac{V_{OC} \times J_{SC} \times FF}{P_{in}} \]

The reduction of FF will significantly drop the device efficiency ! ! !

(ii) Appearance of S-shape in OPVs and possible mechanisms

<table>
<thead>
<tr>
<th>Polymer BHJ</th>
<th>Dipole</th>
<th>Electrode degradation</th>
<th>Injection barrier</th>
<th>Charge accumulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small molecule PHJ</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>?</td>
</tr>
<tr>
<td>DSSC</td>
<td>✔</td>
<td>✔</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

B. Device structure

Devices were fabricated by thermal evaporation under < 1×10⁻⁶ torr

(ii) Appearance of S-shape in OPVs and possible mechanisms

The exact mechanism in PHJ device is still unclear ! ! !

C. Open circuit voltage and fill factor varies with BPC thickness

(ii) Appearance of S-shape in OPVs and possible mechanisms

Bathocuproine (BCP)

(i) Charge accumulation at the C60 and BCP interface

(ii) Gaussian distributed gap states in the BCP → pinning of Fermi level.

D. Simulation of S-shape effect

(i) Band diagram of the simulation model

(ii) Parameters used in simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Numerical value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bandgap</td>
<td>(E_{gA}), (E_{gD})</td>
<td>1.7 eV, 1.7 eV, 1.4 eV</td>
</tr>
<tr>
<td>Electron mobility</td>
<td>(\mu_e)</td>
<td>10⁻² cm²/Vs</td>
</tr>
<tr>
<td>Hole mobility</td>
<td>(\mu_h)</td>
<td>10⁻² cm²/Vs</td>
</tr>
<tr>
<td>Eff. density of states</td>
<td>(N_e), (N_h)</td>
<td>1.7×10¹⁵ cm⁻³</td>
</tr>
<tr>
<td>Dielectric constant</td>
<td>(\varepsilon_r)</td>
<td>4</td>
</tr>
<tr>
<td>Injection barrier</td>
<td>(\Phi_{in}, \Phi_{out})</td>
<td>0 eV, 0.1 eV</td>
</tr>
<tr>
<td>Temperature</td>
<td>(T)</td>
<td>300K</td>
</tr>
<tr>
<td>Thickness of organic semiconductor</td>
<td>(L_1, L_2, L_3)</td>
<td>20 nm, 50 nm, 45 nm</td>
</tr>
<tr>
<td>Contact recombination rate</td>
<td>(S_{recA}, S_{recD})</td>
<td>10¹⁰ cm⁻² s⁻¹</td>
</tr>
<tr>
<td>Discrete donor-like</td>
<td>(\sigma_d)</td>
<td>10¹⁰ cm⁻³ s⁻¹</td>
</tr>
<tr>
<td>Gap state concentration</td>
<td>(\sigma_g)</td>
<td>10⁻² cm⁻²</td>
</tr>
<tr>
<td>Capture cross section</td>
<td>(\sigma_c)</td>
<td></td>
</tr>
</tbody>
</table>

E. Conclusion

The origin of S-shape in J-V curves was investigated by inducing it experimentally and theoretically. The charge accumulation induced S-shape J-V curves can be simulated by increasing the buffer layer thickness.

By considering the direct and indirect recombination, the S-shape J-V curves can be simulated by increasing the buffer layer thickness.

E. Conclusion

The origin of S-shape in J-V curves was investigated by inducing it experimentally and theoretically. The charge accumulation induced S-shape J-V can be viewed as an interfacial recombination modulation's result.

Acknowledgements

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References

[1] AMPs-1D approach is developed by Prof. S. J. Fonash and his students at The Pennsylvania State University.
Enhance the light absorption, other than using the tandem and multiband structures.

(i) Tandem
(ii) Multiband

Both enhancements are attributed to the $V_{oc}$ improvement. In our case, we design a multijunction for the short circuit current density ($J_{sc}$) improvement in planar organic solar cells.

Extra absorption in the 340-440nm contributes to EQE enhancement $\Rightarrow$ charge generation !!!

Enhanced optical absorption from 340nm to 440nm, contributed by the absorption of TTPA

Different from the previous findings related to Förster resonant energy transfer due to strong overlapping of emission and absorption, the enhancement in our multijunction devices is correlated to extra free charges generation and transfer. Our findings show that an alternative method to enhance solar spectra absorption by carefully designed band alignment for efficient charge transport throughout device.

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References