The Multi-Particle Drift-Diffusion Approach for Optoelectronic Devices

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The traditional approach for semiconductor transport modeling in electronic devices is typically based on the drift-diffusion model [1], that describes uniquely the electron and hole flux driven by the gradients of the respective thermodynamic potentials, where each particle is assumed in local thermal equilibrium with the host material. Despite it has been the most used approach for electronic device simulation during the last fifty years, the classical drift-diffusion model exhibits several limitations when considering some mechanisms that occur in new nanoscale optoelectronics devices. We developed a novel generalized multi-particle drift-diffusion (mp-DD) model capable to overcome the limitations imposed by the classic drift-diffusion model. It was designed as flexible and reusable tool that takes into account explicitly multiple carrier populations, whether charged and neutral, allowing to consider also e.g. exciton transport or ionic motion, crucial for a relevant number of device structures. The modeling approach provides first of all the generalization to more than two carrier populations, each one individually assumed in a local thermodynamic equilibrium and characterized by its individual electrochemical potential; secondly, the particles are coupled to each other by recombination-generation terms, formulated to be strictly thermodynamically consistent. Figure 1 shows schematically the basic assumption behind the intra-band and inter-band recombination modeling. [2]

We applied the multi-DD in different application contexts. We calculated the impact of intermediated band charge transport on intermediate band solar cell (IBSC) performance, as show in Figure 2. We also model the optical and electrical operation of a thermally activated delayed fluorescence (TADF) in OLED. This represents a good demonstration of how the explicit inclusion of excitons, within the system of equations, allow us to draw important conclusions about the device emission profile (see Figure 3), accounting for typical exciton quenching processes such as triplet-triplet annihilation (TTA) [3] and triple polaron quenching (TPQ) [4].

[1] W. van Roosbroeck et al., Bell Syst. Tech. J., **4(29)**, 560-607 (1950).

[2] D. Rossi et al., IEEE Trans. Electr. Dev., submitted (2019).

[3] H. Uyoma et al., Nature, **7428(492)**, 234 (2012).

[4] M. A. Baldo et al., Phys. Rev. B, **62**, 10967-10977 (2000).

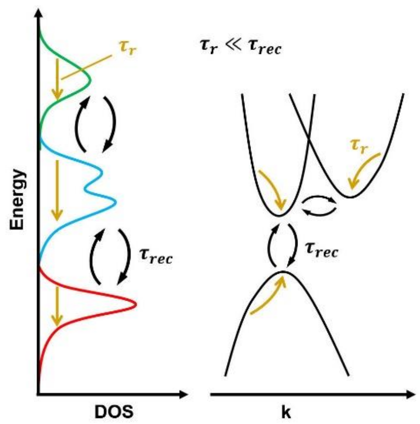

Fig.1: Sketch of the basic assumption in mp-DD model: several particle populations exist (e.g. in different bands, as shown on the right), which are in individual local thermal equilibrium and weakly coupled with each other. τ_r and τ_{rec} represent the characteristic intra-band (relaxation) and inter-band (recombination) scattering times.

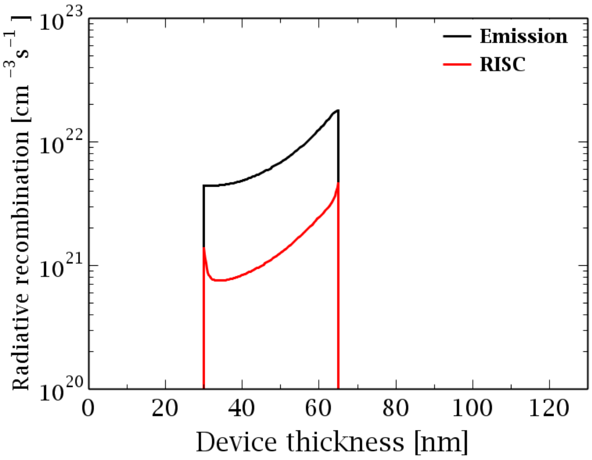

Fig.3: Radiative emission profile (black) and reverse inter-system crossing rate (red) calculated with mp-DD simulation at 6V bias operation within the emitter of a TADF OLED consisting of a TCTA/CBP:4CzIPN/TBPi stack.

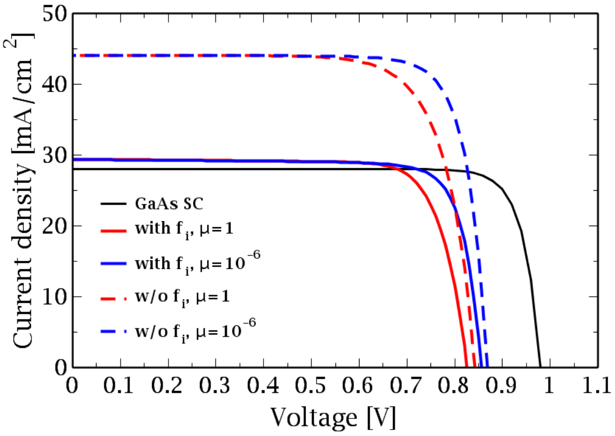

Fig.2: J-V characteristics comparison between experimental results on GaAs based solar cell and on GaAs based IBSC simulations for different electron mobility within the intermediate band (IB). Furthermore, we calculated the carrier generation by absorption accounting (full-lines) and neglecting (dashed lines) the actual occupation of VB,CB and IB.