Recombination in organic solar cells

1) Langevin recombination

Recombination in low mobility semiconductors can be described by Langevin recombination in the form R=knp, where k is the recombination pre-factor and n/p are the free carrier concentrations.

a) Derive the Langevin prefactor k – show all the steps of your derivation and write one sentence for each step describing the physical meaning of the step.

b) The value of k measured in P3HT:PCBM is often up to 1000 times smaller than that predicted by pure Langevin recombination.   What other evidence is there that the simple Langevin recombination model may not be a good model for recombination in P3HT:PCBM? (Please cite the paper which contains the information in your answer)

2) Shockley-Read-Hall (SRH) recombination
a) Draw and label a diagram depicting SRH recombination for a single trap level.

b) Write the equation for free electron capture into the electron trap state and name each term.

c) Write the equation for trapped electrons escaping into the free carrier population and name each term.

b) Due to the principle of detailed balance, in thermal equilibrium each carrier trapping and de-trapping process must balance. By setting the electron capture rate into an electron trap equal to the electron escape rate from the electron trap ($r_1=r_2$), by using the Fermi-Dirac distribution

$$f = \frac{1}{1+\exp\left(\dfrac{E_t - E_f}{kT}\right)}$$

and the Maxwell-Boltzmann expression for free electrons, show that the escape rate is given as

$$e_n = v_{tv}\,\sigma_n\,N_c \exp\left(\frac{E_t - E_c}{kT}\right)$$, where E_c is the band edge and E_t is the trap level.

c) Both carrier dependent Langevin recombination (MacKenzie et al. *J. Phys. Chem. C*, 2011, 115 (19), pp 9806–9813) and SRH recombination (Kirchartz et al. Phys. Rev. B 83, 115209 (2011)) can be used to describe recombination in OPV devices. In SRH recombination carrier recombine via a trap state, thus recombination can be though of as free carrier to trapped carrier recombination. Show that carrier density dependent Langevin recombination is equivalent to free-carrier to trapped-carrier recombination.

d) Carrier dependent Langevin recombination assumes that all the carriers have had time to thermalise and thus assumes one quasi-Fermi level can describe both free and trapped carriers. Under which circumstances may this not be a good approximation?

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