Kinetic Monte Carlo Simulation of Molecularly Doped Organic Semiconductors

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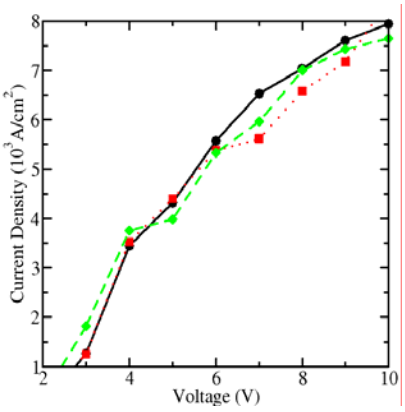
Novel optoelectronic devices are assemblies of ~100 nm thin functional organic layers of an appropriate crystallographic phase. Electric current shows an activated, barrier-crossing behavior furnishing the carrier mobility with a Poole-Frenkel-type field dependence and a carrier concentration dependence able to differ for diluted (OLEDs) and dense (OFETs) electron gases for one and the same polymer (1). The polaronic degree of the transport mechanism's nature depends on two main sources of spacial correlations: the film's morphology and its molecular structure. Simulations allow us to vary parameters and to study otherwise unaccessible conditions. If transport, recombination, generation, injection, ejection, and space charge are captured consistently, the relevant transport data are accessible under a variety of field conditions. In this spirit, an unipolar kinetic Monte Carlo simulator applicable to all morphologies has been developed. Emanating from Bässler's explanation of Gill's law, Miller-Abrahams jumps in an otherwise static set of strictly localized states have been assumed. The resulting biased random walk covers many important features of energetic and positional disorder, provided that the state-energies are (i) spacially uncorrelated, (ii) Gaussian distributed, and (iii) represent the sole origin of activation energy (2). The simulator operates simultaneously on bonding as well as antibonding hard, i.e. constantly repulsive, π-electrons obeying fermionic exclusion. Drift, diffusion, generation and recombination with vacancies all take place on a microscopic time-scale, where no two Metropolis-sampled events may occur at the same time. The lack of intrinsic electrons focussed attention on samples doped with thermally exciteable shallow traps. Carrier injection and ejection at the contacts has been integrated into the bulk dynamics. The frequently assumed periodic boundary conditions have been abandoned to cover boundary and interface effects. Molecules have been modeled as particle-resevoirs mirroring the molecule size. Our attempts (Figure) to reproduce the current-voltage characteristics of amorphous ZnPc:0.3%F_4TCNQ measured by (3) for 5, 10 and 15 % Gaussian spacial disorder show that this approach establishes a promising way of simulating the effects of morphology, doping and carrier concentration, all on a common footing.



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References

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