Monte Carlo Simulation of Molecularly Doped Organic Semiconductors

Gregor Meller, Ling Li, and Hans Kosina

Institute for Microelectronics, TU Vienna, Gußhausstraße 27–29, A-1040 Wien, Austria
Phone: +43-1-58801/36017, Fax: +43-1-58801/36099, Email: meller@iue.tuwien.ac.at

Novel electronic and optoelectronic devices like organic field-effect transistors and light emitting diodes consist of thin amorphous or polycrystalline films with a thickness of about 100 nm. Charge transport strongly depends on the film's morphologic and molecular structure and exhibits various regimes. Small polaron transport in narrow bands might occur at very low temperatures in highly ordered organic crystals, whereas pure hopping between strongly localized states is typical for amorphous layers of small, evaporable molecules. Polymers constituted by chains may be viewed as an intermediate stage. Although their susceptibility to traps is high when disordered, proportional to the degree of ordering a decreasing excitonic binding energy is observed, indicating an enhanced delocalization along the polymer backbones. Charge transfer between chains in turn shows typical hopping behavior.

Current transport in random organic media can often be described by the variable range hopping model within an exponential density of states [1]. However, as illustrated in [2], amorphous layers of small molecules are better described by a gaussian energetic disorder. This corresponds to the assumption that all electrons are localized which formed the basis for our Monte Carlo approach.

Since the intrinsic conductivity of disordered organic systems lies usually several orders of magnitude below that of metals, controlled doping by coevaporation with organic π-electron acceptors or donors of low molecular weight is employed to improve conductivity and reproducibility.

We simulated thermally assisted tunneling in doped disordered films of small molecules. Our aim is to reproduce the experimental data for p-doped zinc-phtalocyanine presented in [3]. Employing a gaussian density of states, these data have been discussed on the grounds of the transport-energy concept [4]. Besides the mobility's temperature and field-dependence we want to study the influence of the carrier concentration, the host's crystallographic phase and the system's doping level. The simulator is capable of simultaneously covering the drift, the excitation and the recombination of carriers at arbitrary doping-levels and carrier-concentrations. In the style of [2], the carrier energies have been assumed to be smeared around the highest occupied bonding and the lowest unoccupied antibonding level. We started with an Abraham-Miller-like tunneling mechanism [5] to mimic the electron transfer among the molecules and incorporated the different size of dopand- and host molecules. The electrons obey the fermionic exclusion principle thus experiencing a pairwise repulsion. The system dynamics is modeled semi-markovian, hence as suggested in [6] the system-time is incremented by non-uniform steps mirroring a hierarchy of (Metropolis-sampled) events, in which solely the fastest event within the system is realized giving rise to a new configuration. In this way, different time-scales corresponding to inter- and intra-molecular events are handled consistently. Inspired by [7] we included the electrodes as jumping-sites settled at the corresponding boundarys of the system. Hence injection and ejection of carriers are incorporated into the dynamics. The injection barrier is modeled as the sum of a zero-field barrier and the injected electron's image charge. This work shows a promising way for the simultaneous simulation of morphology, doping, and carrier concentration effects on the local mobility distribution and the system's current-voltage characteristics.

REFERENCES

[1] M.C.J.M.Vissenberg and M.Matters, Phys.Rev.B **57**, 12964 (1998).

[2] H.Baessler, Phys.Stat.Sol.(b) **175**, 15 (1993).

[3] B.Maennig *et al.*, Phys.Rev.B **64**, 1952081 (2001).

[4] R.Schmechel, J.Appl.Phys. **93**, 4653 (2003).

[5] A.Miller and E.Abrahams, Phys.Rev **120**, 745 (1960).

[6] L.A.Ray and R.C.Baetzold, J.Chem.Phys. **93**, 2871 (1990).

[7] U.Wolf, V.I.Arkhipov, and H.Bassler, Phys.Rev.B **59**, 7507 (1999).