Monte Carlo simulations of charge transport in organic solar cells

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We report random walk Monte Carlo simulations of transient currents in polymer semiconductors of the type used in organic solar cells and compare our results with experimental time of flight (ToF) data. In these experiments, a pulse of light incident on the organic material near one electrode (the choice of electrode determines the carrier type studied) generates a thin sheet of charge carriers that drifts under an applied field to the collecting electrode [1]. The carrier mobility μ is deduced from the transit time for the charges across the sample and can be obtained from the transient currents [1].

Our simulations assume that the material can be considered as a collection of hopping sites for charges. The hopping sites are rods representing conjugated polymer segments as shown in Fig 1 for the morphology used in Fig 2. Periodic boundary conditions are applied in the *y* and *z* directions. In other simulations, we have varied the rod orientations such that the chains are set to be parallel with the *y* axis, while in the centre of the device their orientation becomes much more random, and they have been specified as being fairly rigid, ie neighbouring rods only differ in alignment by a small angle. The energies associated with each segment are assumed to vary as a Gaussian distribution of width α. Explicit allowance is made for the displacement current. An advantage of our approach with an explicit albeit simplified morphology is that it is readily generalisable to polymer blends and to exciton diffusion.

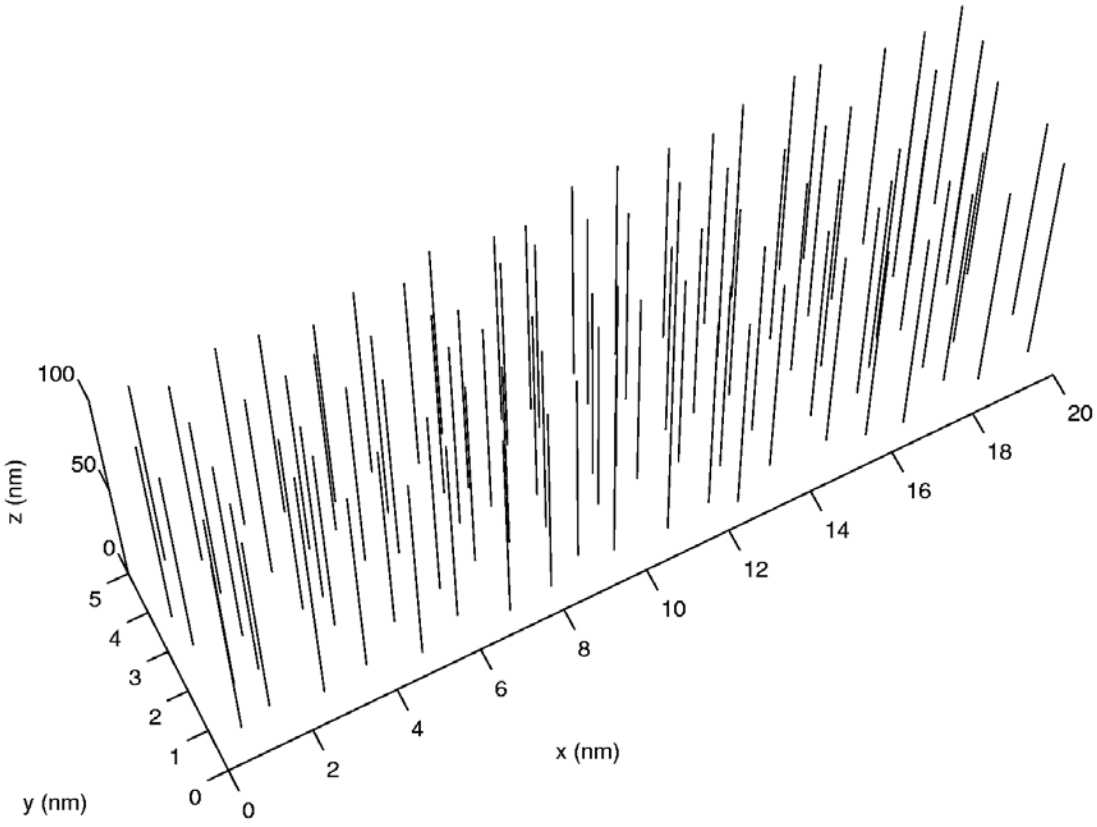

Figure 1. Diagram showing the linked segments representing conjugated polymer chains in the Monte Carlo simulation (only a small portion of the model system is shown for clarity).

Simulations have been repeated with varying field, temperature and sample morphology and the effect of these parameters established. In most Monte Carlo simulations of organic

semiconductors, including ours, the jump rate from a site to the neighbouring site is assumed to take a semi-phenomenological Miller-Abrahams form. The work presented here is a development of earlier work by us [2], but here a more realistic description of the morphology has been achieved. Examples will be shown at the conference where the morphology and energy distribution of the conjugated segments is varied. Characteristics which can be varied are: the preferred orientations of chains, the extent to which they conform to this orientation, the rigidity of chains and the number and length of segments.

In Fig 2 the predicted variation of $\log(\mu)$ with the square root of the applied field $E^{1/2}$ is shown for different temperatures. The morphology used was that of aligned, but randomly translated chains as shown in Fig 1, and the energetic disorder width was $4k_BT$ where k_B is the Boltzmann constant and T the temperature

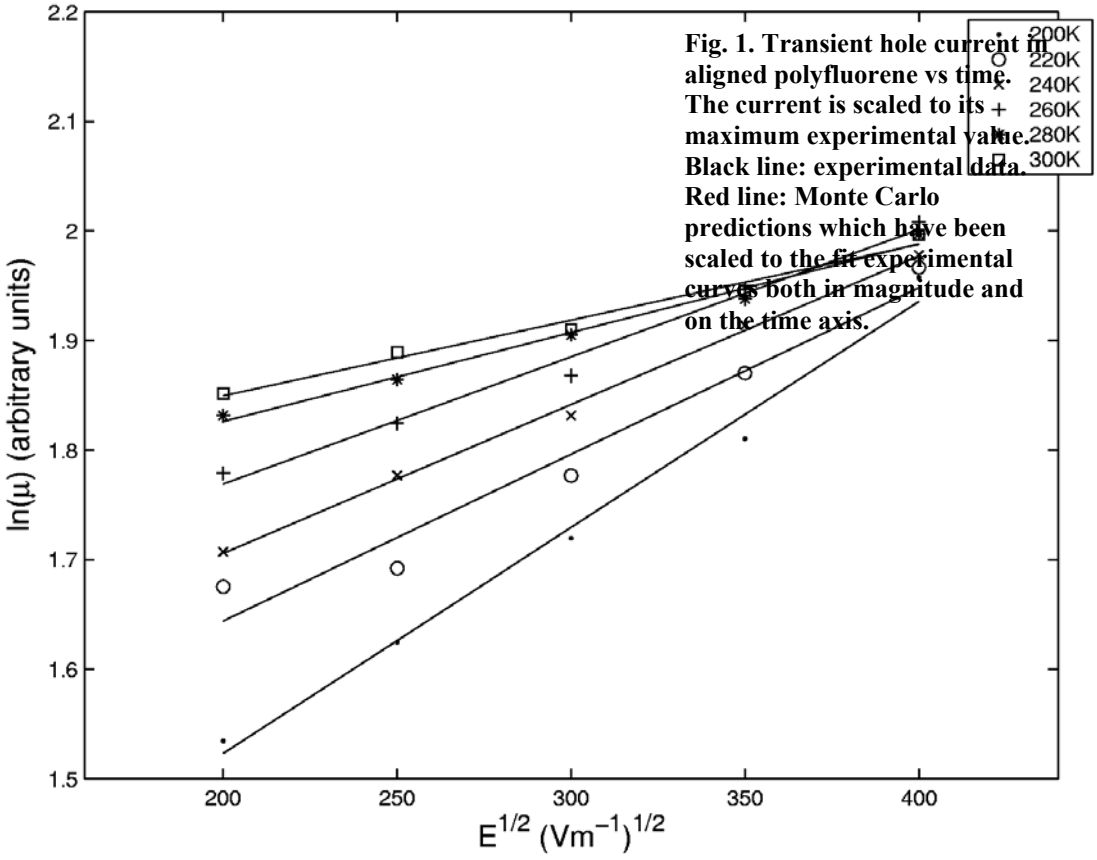

Fig. 1. Transient hole current in aligned polyfluorene vs time. The current is scaled to its maximum experimental value. Black line: experimental data. Red line: Monte Carlo predictions which have been scaled to the fit experimental curves both in magnitude and on the time axis.

There is agreement in that both model and experiment show a linear dependence of $\log(\mu)$ on $E^{1/2}$ with a positive gradient, and also increasing mobility with temperature. Model and experiment differ in that the effect of temperature on $\log(\mu)$ is orders of magnitude greater in experiment, and the gradient of the $\log(\mu)$ vs $E^{1/2}$ plot is independent of temperature in the experimental data, but decreases with temperature in the model.

References

1. A B Walker, A Kambili, S J Martin "Electrical Transport Modelling in Organic Electroluminescent Devices" Review, J. Phys.: Condens. Matter **14** 9825 (2002)
2. S J Martin, A Kambili, A B Walker "Temperature and Field Dependence of the Mobility of Highly Ordered Conjugated Polymer Films" Phys Rev B **67**, 165214, (2003)