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Original Paper

Analysis of charge transient spectroscopy data originating from Gaussian densities of electron states in organics

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Abstract

For a large number of organic disordered semiconductors the transport of electrons or holes via hopping is mediated by localized states in the band gap. An attempt is presented towards testing the widely met hopping transport model based on the assumption of a Gaussian density of states (DOS). An analysis of both isothermal and thermal charge transient spectroscopy (QTS) response to recharging the Gaussian DOS by a sudden change in the applied bias (pulse) is presented. A three-channel correlator is used for processing the exponential decay of transient charge $Q(t)$ *after* the pulse: $\Delta Q = Q(t_1) - 3/2Q(2t_1) + 1/2Q(4t_1)$, the response ΔQ peaking at the delay $t_{1\max} \approx \tau_i$, the latter quantity standing for the time constant of recharging the i-th level of a discrete Gaussian spectrum of electron states. It is shown how the variances w of the isothermal ΔQ-$\log_{10}(t_1)$ spectrum and w_T (in K) of a thermal ΔQ-T peak ($T \longrightarrow$ temperature) are transformed to the variances in energy σ and σ_T, respectively. For the isothermal regime there is an analytical expression for the error of the transform due to the finite energy resolution of the ΔQ filter of time constants, however, the error in σ_T is to be assessed via simulation. Practical usage of the formalism is exemplified, taking QTS spectra of Ag/Dimethyl-PTCDI/GaAs diodes as reference. The dominant peak (0.26 eV) is assigned to a dielectric relaxation, i.e. to charging the depletion layer capacitance of GaAs through the equivalent parallel resistance of the organic layer. In addition, QTS responses of metal/Alq_3/indium-tin-oxide diodes are analysed, Alq_3 being known as a prototypic disordered organic material with hopping transport of electrons *via* localized states in the band gap. In the latter case two processes have been envisaged, assigned to hopping of free charge carriers (signal tail at short times) and a distributed dielectric relaxation peak, respectively. This is to be compared with the case of locally ordered Alq_3 layer on the same substrate, the QTS spectrum comprising three linear

relaxation processes characterized by discrete time constants, while the signal tail pointing to the hopping transport being absent. The linear dependence of the peak heights on both the excitation pulse amplitude and polarity is suggestive of the presence of "dipolar" defects, envisaged as rotating polar molecules. The relative density of these (polarization) is peaking in the nitrogen-rich Alq_3 thin films.

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