Small Polaron Hopping Transport in 1D Disordered Systems

G.P. Triberis and **M. Dimakogianni**

University of Athens, Department of Physics, Solid State Section,

Panepistimiopolis, 157 84, Zografos, Athens, Greece

The electrical transport properties of disordered materials has been an active research topic for many years. The realization of innovative applications in nanotechnology has especially generated a widespread interest on the transport properties of 1D systems, such as carbon nanotubes, nanowires and conducting molecules, with DNA being placed among the most promising materials.

According to percolation theory the investigation of charge transport in disordered systems is equivalent to the study of the possibility of the passage of the carriers through a random network of impedances which interconnect the different lattice sites. The presence of disorder, under certain circumstances, induces localization of the carriers and hopping is the responsible transport mechanism for the measured conductivity. If the interaction of the carriers with the "lattice sites" is strong enough, it may result in a binding energy larger than the bandwidth, i.e. a polaron is expected to be formed.

Triberis et. al. [1, 2] investigated small polaron hopping transport in 1D disordered systems, such as DNA, at high temperatures (h), ignoring the effect of correlations. An analytical expression for the temperature dependence of the electrical conductivity, $\ln\sigma^{h}\sim T^{-2/3}$, was obtained. The theoretical analysis was based on the Generalized Molecular Crystal Model (GMCM) introduced by Triberis and Friedman [3], appropriate for the study of small polaron transport in disordered systems, the Kubo formula and theoretical percolation arguments.

When the site energies are not the same, the energy of a site affects the incoming as well as the outgoing impedances connected to the given site, and this gives rise to correlations between neighbouring impedances. Recently, Triberis and Dimakogianni [4, 5] showed that the inclusion of correlations (cr) leads to a $\ln\sigma^{h,cr}\sim T^{-1/2}$ law. Their results reproduced satisfactorily the experimental data reported for λ-DNA and for poly(dA)-poly(dT) DNA [6,7,8], considering DNA as a disordered molecular wire. The maximum hopping distances evaluated support the idea of long distance charge migration in DNA.

Triberis and Dimakogianni [9] also examined the interplay of the electric field, F, and the temperature on the small polaron hopping conductivity of 1D systems, ignoring correlations. For the high-T regime (h), they obtained $\ln\sigma^{h}(F,T)\propto -T^{-2/3}[1-F^{2}/g(T)]^{1/3}$, where $g(T)=(2\alpha k_{B}T/e)^{2}$ and α^{-1} is the spatial extent of the electronic wavefunction, while for the low-T regime (l) $\ln\sigma^{l}(F,T)\propto -T^{-1/2}[1-F^{2}/g(T)]^{1/2}$.

Most recently, Dimakogianni and Triberis investigated the effect of correlations on the field- and temperature- dependence of the small polaron hopping conductivity. For the high- and low-T regime, and up to moderate electric fields, the small polaron correlated hopping conductivity was found to follow $\ln\sigma^{cr}(F,T)\propto -T^{-1/2}[1-F^{2}/g(T)]^{1/2}$.

The analytical expressions obtained were applied to experimental findings concerning charge transport in Polydiacetylene quasi-1D single crystals [10]. It was shown that the electric

field and the temperature act competitively upon the behavior of the electrical conductivity, and their effect on the transition from the omhic to the non-ohmic behavior of the conductivity, as well as the effect of correlations, was revealed.

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