Polaron Hopping in Nano-scale Poly(dA)-Poly(dT) DNA

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We investigate the current-voltage relationship and the temperature dependent conductance of nano-scale samples of poly(dA)-poly(dT) DNA molecules. A polaron hopping model has been used to calculate the I-V characteristic of nano-scale samples of DNA. This model agrees with the data for current vs. voltage at temperatures greater than 100K. The quantities G_0, i_0, and T_{1d} are determined empirically and the conductivity is estimated for two samples of poly(dA)-poly(dT).

We consider that charge carriers are localized on a base pair and interact with phonons generated by motions in the double helix. This interaction leads to the formation of a localized polaron, whose states are distributed randomly in energy and space coordinates [1]. Polarons move throughout the DNA molecule by random hops in this "hopping" space. The transition rates for these polarons are calculated based on the work of Emin [4]. The recent work of Singh [1] develops a theoretical approach to the phonon-assisted hopping conduction mechanism of polarons in DNA, based on the general molecular crystal model employed by Triberis and Friedman [5]. By treating DNA as a quasi-one dimensional molecular crystal, a 2/3 power law for the temperature dependence for the conductivity is developed and is found to agree well with the experimental results of Kutnjak et al. [1,3].

In this study, we extend the work of Singh [2] to develop a model to explain the nonlinear current-voltage relationship for poly(dG)-poly(dC) and poly(dA)-poly(dT) DNA molecules, using a 2/3 power law for temperature. A good agreement is found between the model and data obtained from Yoo et al. [2]. The 2/3 power law is used to obtain the fitting parameter $T_{d,}$ which contains information about the density of states in the DNA, from the temperature dependent conductance. This value is, in turn, used to find the characteristic current i_0 and temperature dependent polaron hopping distance *a* from the I-V curves of poly(dA)-poly(dT) at 161K and 223K. We find that our analysis yields a nonlinear hopping distance in temperature, which warrants a more detailed study.

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