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Collective Charge Transport in a Chain of Graphitized Carbon Nanoparticles

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We carry out Monte Carlo dynamics simulations to study the current-voltage (I-V) characteristics of one-dimensional arrays of nanoscale particles coupled by tunneling with random offset charges. The present model system is found to exhibit a voltage-driven phase transition under appropriate conditions from a insulating state to a conducting state, which is characterized by a threshold behavior of I-V curves and also a scaling behavior of the current above the threshold voltage. The results agree well with recent experiments on a chain of graphitized carbon nanoparticles.

Keywords: carbon nanoparticle; charge transport; threshold behavior; tunneling

INTRODUCTION

Over the past several years, there is a huge interest on transport properties of one- and two-dimensional arrays of nanoscale particles coupled by tunneling [1]. It is because such arrays exhibit a voltage-driven phase transition between static (nonconducting) and dynamic (conducting) states, which is characterized by the threshold behavior of current-voltage (I-V) characteristics. Indeed, these threshold properties have been applied for construction of nanoscale electronic devices such as single electron transistors. Recent experiments have revealed

that the threshold behavior of I-V characteristics can be understood as the collective charge transport phenomena due to a correlation between the tunneling acts of individual electrons under the influence of their Coulomb interaction (the Coulomb blockade) and/or charged impurities trapped in the substrate [1].

To raise the efficiency of electronic memories applying the threshold properties, it is necessary to fabricate very small tunnel junctions with small capacitance and large resistance. Indeed, to realize the sharp onset of conduction even at finite temperatures, a small capacitance is needed for large values of Coulomb charging energy, while a large resistance is required to ignore the quantum tunneling effect [1]. Currently, to attain this purpose, a single chain of graphitized carbon nanoparticles has attracted much attention as a desirable system [2]. This system is composed of graphite nanoparticles with the size $\sim$30 nm in diameter having small capacitance ($C \sim 10^{-18}$ F) and high tunneling resistance ($R \sim 10^{9}\Omega$). As a result, the threshold behavior of this system has been observed up to relatively high temperature $T_{th} \sim 77$ K with the large threshold voltage $V_{th} \sim 0.4$ V at zero temperature T=0 K. Note that typical values of these quantities for other systems are $C \sim 10^{-15}$ F, $R \sim 10^{6}\Omega$, $T_{th} \sim 10$ K and $V_{th} \sim 0.01$ V, respectively [3].

Motivated by the above experimental results, we here report the I-V characteristics in such a chain numerically on the basis of Monte Carlo simulations of a simple but commonly accepted model [1]. The original model has been proposed by Middleton and Wingreen (MW), which is valid only in zero temperature limit [4]. Thus, we here extend the MW model to include the thermal fluctuation effects on the tunneling behavior. In addition, we examine effects of the impurity strength on the threshold voltage, which has been less studied.

THE MODEL

Here we consider a one-dimensional array of N nanoparticles which bridges the gap between two electrodes (leads), linked by tunnel junctions of resistance R and capacitance C and located close to a ground plane to which each particle has a capacitance C_g. The leads are taken to have infinite self-capacitance and

have a capacitance C to adjacent particles. We assume that the tunnel resistance R is larger than the quantum resistance $R_Q \equiv h/(2\pi e^2)$ and the charging energy $e^2/(2\max[C, C_g])$ is larger than the thermal energy kT, with an elementary charge e, Planck constant h, and Boltzmann constant k. An electrostatic energy of the system can be written in the form [4]

$$E = \frac{C_g}{2}\sum_{i=1}^{N} v_i^{\,2} + \frac{C}{2}\sum_{i=0}^{N}(v_{i+1} - v_i)^2 \tag{1}$$

where v_i are the electrochemical potential of the i-th particle and are expressed in terms of the electric charges as

$$-Cv_{i-1} + (2C + C_g)v_i - Cv_{i+1} = Q_i + q_i . \tag{2}$$

Here, $Q_i = -n_i e$ is the net mobile charge with an integer n_i located in the site i, while q_i represents a offset charge in the i-th particle induced by charged impurities trapped near the particle-substrate interface which acts as a quenched disorder and is characterized by Gaussian random numbers with zero mean and standard deviation $e\sigma$.

We study the current-voltage (I-V) characteristics of the above model numerically by using classical Monte Carlo (MC) nonequilibrium dynamics, regarding the MC time as real time [5]. This should be a reasonable approximation in the overdamped limit and when quantum effects can be ignored, as the case considered here. The voltage biased array is realized such that the left lead potential v_0 is fixed to be a bias voltage V, and the right lead potential v_{N+1} to be zero, respectively. Simulation procedure is as follows [6]: Choosing a nearest neighbor pair (i,j) at random, we try to increase n_i by 1 and decrease n_j by 1, thus transferring an electron from j to i. Following the heat bath algorithm, if the change in energy is ΔE, the move is accepted with the probability $1/(1+\exp[\Delta E/(kT)])$. The applied voltage V gives an electric potential $-eV$ on an electron. The potential can be incorporated into the Monte Carlo moves by adding to ΔE an amount eV if the electron moves in the direction opposite to the electric force, and subtracting this amount if it moves in the same direction. Biasing the moves in this way takes the system out of

equilibrium and causes a net current across the system in a direction along the bias voltage, calculated by

$$I(t) = \frac{1}{N\Delta t}\sum_i \Delta Q_i(t) \tag{3}$$

where t denotes a MC time (incremented by Δt after each attempted move), and $\Delta Q_i(t) = e$ if an electron at site i moves one lattice spacing in the direction of the electric force at time t, $\Delta Q_i(t) = -e$ if the electron moves in the direction opposite to the electric force. We set $\Delta t = 1/(2N)$ so that an attempt is made to move each electron once in each direction, on average, per unit time. Initially, we set $Q_i = 0$ for all particles.

SIMULATION RESULTS

We simulate the collective charge transport phenomena of the extended MW model when the biased voltage V is applied, by changing values of temperature T, chain size N, capacitance ratio C/C_g, and impurity strength σ. In the following simulations, we take the unit of energy to be $E_0 = e^2/(2C_g)$, temperature to be $T_0 = E_0/k$, and voltage to be $V_0 = e/(2C_g)$, respectively.

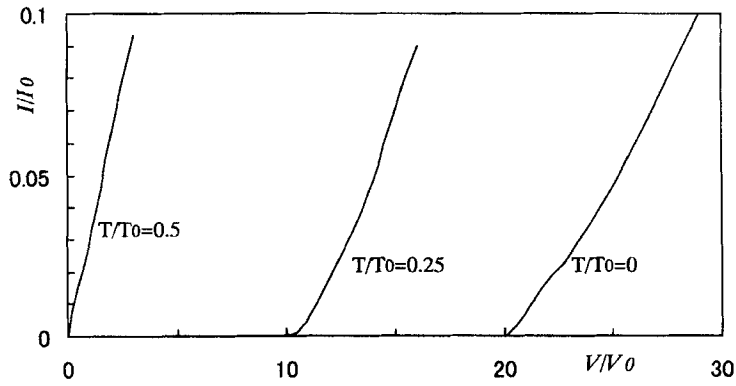

FIGURE 1 Temperature dependence of I-V curves

In Fig.1 we show the I-V curves for three values of temperature with $\sigma = 0.01$, N=40, and $C/C_g = 2.35$, which are measured by experiments in the array of carbon nanoparticles [2]. We use the unit of current to be $I_0 = 10^{-6}V_0/R_q$. From this figure we can see that the model exhibits a phase transition between the insulating state with zero current and the conducting state with finite current for appropriate conditions. The results are in good agreement with the experimental data. For instance, the computed threshold voltages, $V_{th}/V_0 = 20.2$ at $T/T_0 = 0$ and $V_{th}/V_0 = 10.5$ at $T/T_0 = 0.25$, are consistent with the experimental values $V_{th} = 0.4$ V at T=0K and $V_{th} = 0.2$ V at T=60K, respectively, because of $V_0 = 0.02$ V and $T_0 = 231$ K for the array of carbon nanoparticles.

From further simulations of the I-V curves with $100 \le N \le 1000$, we compute the threshold voltage V_{th} and the scaling exponent x, assuming that the current I exhibits the scaling behavior as $I \propto (V - V_{th})^x$ for $V > V_{th}$ [6].

In Fig.2 we show the threshold voltage V_{th} as a function of the capacitance ration C/C_g for three values of the impurity strength at T=0 in a log-log scale. For T=0 and σ =0, it is found that we obtain the results $V_{th} = eN/(2C_g)$ for $C_g \gg C$ and $V_{th} = eN/(2C)$ for $C_g \ll C$, as was expected. In addition, we can see that the threshold voltage gains fairly even for small impurity strength. From more detailed analyses, we have numerically confirmed that the functional form of the threshold can be expressed as $V_{th} = V_0 N[B(C/C_g, \sigma) - kT/(eV_0)]$, where $B(C/C_g, \sigma)$ denotes the threshold voltage at T=0 given in Fig.2.

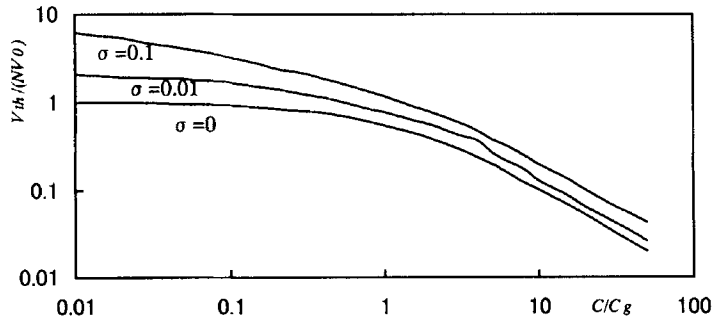

FIGURE 2 Threshold voltage Vth at zero temperature

In Fig.3 we show the scaling exponent x as a function of temperature for three values of the impurity strength. The exponent is found to be an increasing function of both σ and T. We should state that in one-dimensional systems one has obtained x=1 theoretically [1], and $1 \leq x \leq 2.5$ experimentally for graphite particles [2]. It should be noted that within the present simulations no evident dependence of the exponent on N and C/C_g has been observed.

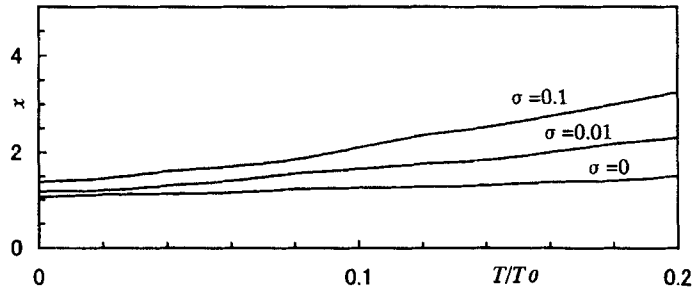

FIGURE 3 Temperature and disorder strength dependences of x

CONCLUSION

We have performed Monte Carlo dynamics simulations of the extended MW model to study the I-V characteristics of the voltage biased one-dimensional array of nanoparticle linked by small tunnel junction with random offset charges. The numerical results by using associated parameters values are in good agreement with recent experimental data for one-dimensional chains of graphite carbon nanoparticles.

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