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Current-voltage characteristics of conducting polymers and carbon nanotubes

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Abstract

The electronic transport properties of a number of materials with nanoscale or microscale structure show some remarkable similarities despite the differing conduction mechanisms expected in different materials, for example similar nonlinearities in their current-voltage characteristics. We propose a generic expression for the nonlinear current-voltage characteristics based on our numerical calculations for metallic conduction interrupted by small barriers. We discuss the general features of the experimental data and show that our expression gives a very good description of the observed nonlinearities in carbon nanotube networks, vanadium pentoxide nanofibres and polyacetylene nanofibres, as well as half-metallic granular Sr_2FeMoO_6 that is of interest for spintronics.

Keywords: Conducting polymers, Carbon nanotubes, Conductivity, Spintronics

1. Introduction

To understand the unusual electronic transport properties of novel materials (especially low-dimensional materials), many different conduction mechanisms have been considered [1]. In quasi-one-dimensional materials, conduction barriers caused by any kind of defect are likely to make a substantial contribution to resistance. In many highly conducting polymers and carbon nanotube networks, the mixed metallic and nonmetallic behaviour of conductivity can be explained in terms of metallic regions or segments in series with barrier regions [2,3].

In this paper, we focus on the current-voltage (*I-V*) characteristics, a key indicator of the electrical behaviour of conducting materials. From our numerical calculations for conduction through small barriers between metallic regions, we infer a generic expression for the nonlinear *I-V* characteristics. We illustrate a striking similarity in the *I-V* characteristics of carbon nanotubes, V_2O_5 nanofibres, polyacetylene nanofibres, and the half-metallic ferrimagnet Sr_2FeMoO_6 (of interest as a possible source of spin-polarized tunnelling currents for spintronics). We show that the *I-V* characteristics of all these materials are in very good agreement with the nonlinearity predicted by our numerical calculations.

2. Calculations

Since the conductivities of highly conducting polymers and single-wall carbon nanotube networks show evidence of metallic conduction interrupted by small barriers, we have used this model as a base for comparison with experimental data on the *I-V* characteristics. We have made numerical calculations of the current due to fluctuation-assisted tunnelling through conduction barriers and thermal activation over the barriers. The mean current density through a barrier when a field E_a is applied across it is evaluated as

$$j(E_a) = \int_{-\infty}^{\infty} dE_T \; j(E_a + E_T)\, P(E_T) \,, \tag{1}$$

where $P(E_T)$ is the probability [4] that the fluctuation field across the junction has the value E_T (which may be in either direction). The tunnelling current $j(E)$ for a total field $E_b = (E_a + E_T)$ in the barrier is given by [4]

$$j(E_b) = \frac{me}{8\pi^2\hbar^3} \int_{-\infty}^{\infty} d\varepsilon \, D(\varepsilon, E_b)\, \Theta(\varepsilon, E_b) \tag{2}$$

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where m and ε are the carrier mass and energy respectively, $D(\varepsilon,E_b)$ is the barrier transmission factor approximated by the usual exponential WKB expression with $D(\varepsilon,E_b) = 1$ for energies ε greater than the top of the tunnelling barrier, and $\Theta(\varepsilon,E_b)$ is the appropriate "supply function" determined by the Fermi factors on each side of the barrier.

We extend Sheng's work [4] to apply to our case by including the backflow current, the tunnelling near the top of the barrier and thermal activation over the barrier, and by performing full numerical calculations rather than making analytic approximations.

For a range of barrier parameters, we find that our numerical calculations of the I-V characteristics are well described by the generic expression

$$G = \frac{I}{V} = \frac{G_0 \exp(V/V_0)}{1 + h\,[\exp(V/V_0) - 1]} . \qquad (3)$$

The meaning of the parameters is as follows. G_0 is the temperature-dependent low-field conductance (the ohmic term as $V \to 0$). The parameter V_0 (which depends strongly on the barrier energy) is the voltage scale factor in the term that gives an exponential increase in conductance as V increases. As the field increases so that the difference in Fermi levels on either side of the barriers is comparable to the barrier energy, the conductance of the material will saturate at a value G_h that reflects the larger conductance in the absence of barriers. The parameter $h = G_0/G_h$ (where $h < 1$) yields a decrease of G below the exponential increase at higher voltages V (the saturation of G at a high-field value G_h as $V \to \infty$ given by Eq. (3) is an extrapolation of the calculations).

It should be noted that the mean field E in the sample is much smaller than the applied field E_a in the barrier, since the voltage drops will be largest across the barriers. Hence the parameter V_0 depends on geometric factors involving the width and separation of the barriers analogous to those discussed earlier in connection with the low-field conductivity [5].

3. Comparison with experiment

We show in Figs 1 – 5 that our generic expression Eq. (3) gives a very good account of the experimental I-V characteristics of single-wall carbon nanotubes (SWCNTs) [6], V_2O_5 nanofibres [7], individual polyacetylene nanofibres [8,9], and granular Sr_2FeMoO_6 [10]. All these I-V characteristics were essentially symmetric upon reversal of the voltage direction, so to show the fits more clearly only positive voltages are used (but including both increasing and decreasing runs). We look at each of these examples in turn.

Lee et al. [6] prepared individual SWCNTs of diameter 1 – 2 nm suspended in parallel between electrodes 300 nm apart. A representative example of the measured I-V characteristics is shown in Fig. 1 with fits to our expression Eq. (3) with parameter $h \approx 0$ (i.e. the data follow a simple exponential increase of conductance G as applied voltage V increases).

The low-field conductance G_0 of this sample decreases substantially as temperature T decreases, in a manner similar to that seen in SWCNT networks and accounted for by the fluctuation-assisted tunnelling model with barriers of energy up to 10 meV [5]. The low-field tunnelling current in this model remains non-zero in the zero-temperature limit, and the overall temperature variation of G_0 is weaker than that for activated conduction.

The value of the voltage scale parameter V_0 was approximately 60 V at $T = 10$ K and somewhat larger for higher temperatures (but not accurately determined since the nonlinearity is small). The linearity of the I-V characteristics for temperatures of 100 K and above is consistent with a lessening of importance of barriers as thermal energy (around 12 meV at 100 K) becomes comparable to the barriers, although data at higher voltages are needed for clear conclusions.

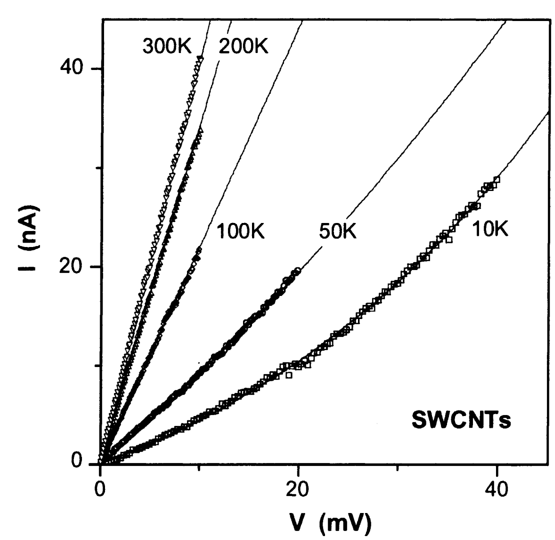

Fig. 1. Current-voltage characteristics of single-wall carbon nanotubes at different temperatures measured by Lee et al. [6], fitted to our expression Eq. (3) for fluctuation-assisted tunnelling and thermal activation (with parameter $h = 0$).

A surprisingly similar pattern is seen in the I-V characteristics of vanadium pentoxide (V_2O_5) nanofibres measured by Kim et al. [7], as shown in Fig. 2. These data are for seven V_2O_5 nanofibres (each with cross-section approximately 1.5 nm by 10 nm) between a pair of electrodes approximately 100 nm apart. The nonlinearities at higher temperatures suggest larger barrier energies than for the SWCNT case. Once again, for these V_2O_5 data, there is no evidence for a deviation from the exponential increase in conductance over the limited range of the measurements. The strong increase of the low-field conductance G_0 in this case was similar to that for activated behaviour (i.e. $\ln(G_0) \propto 1/T$) over this limited range. The voltage scale parameter V_o had values in the range 1.00 ± 0.05 V for the nonlinear data for $T < 200$ K.