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COMMENT

Comment on 'Temperature dependence of the current–voltage characteristics of Sn/PANI/p-Si/Al heterojunctions'

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Abstract

Current–voltage characteristics of Sn/PANI/p-Si/Al heterojunctions, measured in the temperature range 140–280 K by Kaya *et al* (2007 *J. Phys.: Condens. Matter* **19** 406205), are reinterpreted in the framework of phonon-assisted tunnelling theory, as a free-charge-carrier generation mechanism in the strong electrical field. It is shown that phonon-assisted tunnelling more adequately describes the peculiarities of the variation of I–V data with temperature in PANI polymers.

Recently, Kaya *et al* [1] presented current–voltage (I–V) characteristics of Sn/PANI/p-Si/Al heterojunctions, fabricated by electropolymerization of aniline on chemically cleaned p-Si substrates, measured in the temperature range 140–280 K. Analysing the forward bias non-ideal I–V characteristics on a log–log scale, the authors [1] proposed that the space–charge-limited current (SCLC) conduction controlled by an exponential trap distribution (above the valence band edge) dominates the current transport in the PANI/p-Si diodes at high voltages, whereas at low current density thermionic emission over the PANI/p-Si contact is important.

However, the very strong temperature dependence of the barrier height and ideality factor (changing from 0.423 eV and 3.085 at 140 K to 0.716 eV and 1.868 at 280 K, respectively) shows, in the authors' [1] minds, that the forward bias transport properties of the heterojunction diodes are not quite well modelled by the thermionic emission only, and may be a result of other conduction mechanisms.

We suggest that in [1] the observed peculiarities of I–V–T data can be adequately explained on the basis of the phonon-assisted tunnelling model, which has been used successfully to describe the temperature-dependent I–V characteristics and conductivity dependence on temperature not only in PANI films [2, 3] but also in other conducting polymers [4]. Therefore, in this comment we present an alternative explanation of the temperature-dependent nonlinear I–V characteristics of M/PANI/p-Si diodes [1], assuming that the creation of free charge carriers occurs due to phonon-assisted tunnelling from the localized states in the metal–PANI interface.

It is assumed that charge carriers are generated from the electronic states in the polymer near the metal–polymer interface. The electrons enter the conduction band of the polymer as a result of phonon-assisted tunnelling from these levels. In the dc case, these levels are continuously filled from the electrode. The filling process is believed to be very fast, because the thickness for tunnelling is of the order of the atomic size. Assuming that all the released electrons are transferred through the depletion region, the current will be proportional to the tunnelling rate W, i.e. $I = eNWS$, where N is the surface density of localized electrons and S is the area of the barrier electrode. On this basis, we will compare the I–V data extracted from figure 1 in [1] with the tunnelling rate $W(E, T)$.

For computation of the transition rate $W(E, T)$, a relatively simple equation for electron tunnelling from a deep

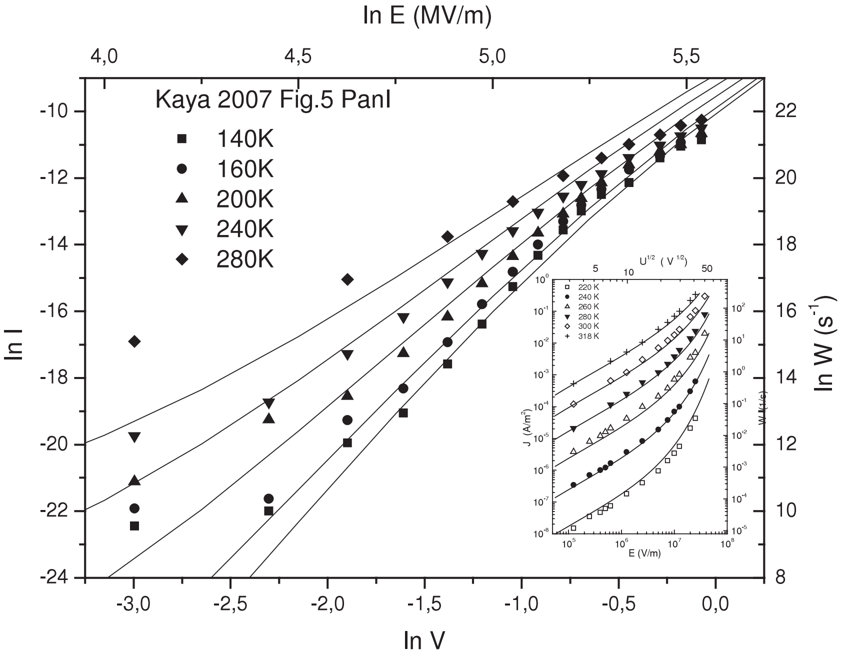

Figure 1. Experimental I–V data of the Sn/PANI/p-Si/Al heterojunction at different temperatures from figure 5 in [1] (symbols) fitted to the theoretical $W(E, T)$ dependences (solid lines) computed using the parameters $a = 9$, $\varepsilon_T = 0.45$ eV, $m^* = 2m_e$, and $\hbar\omega = 12$ meV. In the inset of the figure, the fit of the I–V data of PANI films to $W(E, T)$ from [2] is shown.

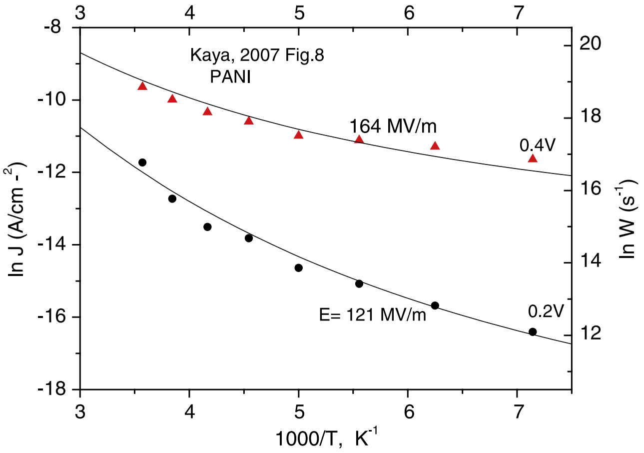

Figure 2. Experimental J versus $1/T$ plot at two voltages from figure 8 [1] (symbols) fitted to the theoretical $W(E, T)$ versus $1/T$ curves computed for the same parameters as in figure 1.

(This figure is in colour only in the electronic version)

centre to the conduction band, presented in [5], is used:

$$W = \frac{eE}{(8m^*\varepsilon_T)^{1/2}}[(1+\gamma^2)^{1/2}-\gamma]^{1/2}[1+\gamma^2]^{-1/4} \times \exp\left\{-\frac{4}{3}\frac{(2m^*)^{1/2}}{eE\hbar}\varepsilon_T^{3/2}[(1+\gamma^2)^{1/2}-\gamma]^2 \times [(1+\gamma^2)^{1/2}+\tfrac{1}{2}\gamma]\right\}, \qquad (1)$$

where

$$\gamma = \frac{(2m^*)^{1/2}\Gamma^2}{8e\hbar E\varepsilon_T^{1/2}}.$$

Here $\Gamma^2 = \Gamma_0^2(2n+1) = 8\alpha(\hbar\omega)^2(2n+1)$ is the width of the centre absorption band Γ_0, being the same at $T = 0$, $n = [\exp(\hbar\omega/(k_B T)) - 1]^{-1}$, where $\hbar\omega$ is the phonon energy, ε_T is the energetic depth of the centre, e is the electron charge, and a is the electron–phonon interaction constant.

The calculation was performed using the effective mass value m^* equal to the free electron mass m_e, and for the phonon energy a value of 12 meV was taken. For the activation energy ε_T, the value of 0.716 eV assessed in [1] was used. The electron–phonon coupling constant a was chosen so as to get the best fit of the experimental data with the calculated dependences, on the assumption that the field strength for tunnelling is proportional to the square root of the applied voltage, i.e tunnelling occurs in the Schottky barrier.

As can be seen in figure 1, the theoretical curves describe the peculiarities of experimental I–V data well enough. The inset of figure 1 shows the fitted I–V data of PANI films to the tunnelling rate computed accordingly to formula (1) from [2]. In this case, an excellent fit of the experimental data to theory for all temperatures has been obtained. It should be noted that the $W(E)$ dependences for different temperatures were obtained using a unique set of parameters, i.e. $a = 9$, $\varepsilon_T = 0.45$ eV, $m^* = 2m_e$, and $\hbar\omega = 12$ meV.

For judgement, the charge transfer mechanism is often carried out considering the temperature dependence of the conductance. In [1] the dependences of current density on the reciprocal temperature of the diodes at various applied voltages are also presented (figure 8) which, in the authors' opinion [1], are straight lines. The ln J versus $1/T$ curves at two values of voltage fitted to the theoretical ln $W(T)$ versus

$1/T$ dependences are presented in figure 2. It is seen that both the theoretical curves and the experimental $\ln J$ versus $1/T$ dependences differ from straight lines, especially at higher temperatures. The nonlinear behaviour of current/conductivity temperature dependence in the Arrhenius plot of polymers and other dielectrics is a well-known phenomenon (see, for example, [6]).

Thus, quantum-mechanical, phonon-assisted tunnelling, as a free-charge-carrier generation process, more adequately describes the peculiarities of the temperature dependence of conductivity and the variation of I–V characteristics with temperature in PANI polymer. Therefore, phonon-assisted tunnelling must be taken into account in describing electrical conductance in polymers, as was described in previous works.

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