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Negative Capacitance Effect Using a Pure Imaginary Electric Mobility Controlled By an Adiabatic Parameter in Thin Film Materials Based On Drude Model

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Abstract

Existence of a pure imaginary mobility of charge carriers in organic polymers materials, precisely the poly p-phenylene vinylene is explored in this work. Indeed, we propose a new model of dynamic equation of particles able to carry electric charges, we introduce a control parameter of the adiabatic evolution combined with a phase difference between the external perturbation of the material and the position of carrier, leading from then on to the non-use of the complex mobility. This model after transformation allowed us to demonstrate the existence of negative capacitance at low and high frequencies in the poly p-phenylene vinylene. Also thanks to this new model, we were able to obtain results in line with the experimental ones, thus confirming the validity of our model.

Keywords: Poly P-Phenylene Vinylene, Pure Imaginary Mobility, Adiabatic Evolution, Negative Capacitance, Organic Polymers.

1. Introduction

Polymer light-emitting diodes and polymer light-emitting electro-chemical cells, are components that have become practically essential in the new miniaturized technologies that are experiencing a meteoric rise [1-8]. This is how organic polymers materials, specifically poly p-phenylene vinylene, are the subject of particular attention regarding studies by an impressive number of researchers following the discovery of the ability of these materials to emit intermittent light after an external disturbance [9]. To better understand the behaviour of these organic polymers, it is necessary to study their characteristics, including the electrical mobility of the charge carriers, which can be electrons, holes, and even both simultaneously although trap-free transport of holes provides a good description of many high-efficiency devices [10-17]. for many of these materials, most of which are disordered, the charge carriers are trapped during their movement in the potential wells found in them, thus constituting a great hindrance to the mobility of the said charge carriers, thus giving them a complex character [18]. Generating more interest, several experimental works have been carried out on the poly p-phenylene vinylene and its derivatives, using as measurement techniques, the current voltage J(V) time of flight (TOF) space charged limited (SCL) and spectroscopic impedance[19-30]. In March 2001, MARTENS et al. in their experimental research on LED polymers, demonstrated the existence of a negative contribution of capacitance at low voltage in these materials [31.32,33]. However, it was only in 2003 that a first theoretical study was carried out by KWOK on LED polymers, confirming the experimental results obtained in 2001 by MARTENS on the capacitance; KWOK thus proposed a first theoretical equation model the development of which led to the experimental results [34]. In this model, it should be noted that one of the constituent parameters of the material, that is mobility, is considered to be a complex quantity, making it difficult to understand. Still based on this model, KWOK carried out several other works [35,36]. Although this model is a pioneer, the fact that the electrical mobility of charge carriers is complex and therefore somewhat nuanced, has opened up research into the existence of a more adequate model. Thus YOU-LIN WU et al in 2019 propose a modified KWOK model, they show that by introducing a phase difference between the electric field and the average position of the charge carrier and by considering the electric mobility this time real, one obtains better results compared to those of KWOK and compared to the experimental results obtained in 2001 by MARTENS et al [37].

Given the increasing importance of imaginary components and their applications, such as the imaginary resistor used by TABUE et al. to manufacture a parity time symmetry dimer, it is therefore appropriate to consider imaginary mobility, since the resistance and electrical mobility of a material are inversely proportional [38]. It is with this in mind that we propose a new model of the dynamics equation that allows us to rigorously obtain the

experimental results with a very low percentage of error.

2. Model and Calculations

Our model consists of an organic polymer of area A and thickness L, containing as carriers of charges holes and electrons.
By considering only, the holes as carriers of charges, and by creating a disturbance in the polymer by means of an external electric field E, the equation of the dynamics reflecting the displacement of the holes and which corresponds to the theory of Drude is given by [34]:

$$m\frac{d^2x}{dt^2}+\frac{q}{\mu^{imag}}\frac{dx}{dt}+K_ox=qE \qquad (1)$$

Where m is the mass of the charge carrier, q the coulomb charge, K_o the Hooke constant, x the average position of the particle and μ^{imag} the imaginary electric mobility of the hole.

Since $P = Nqx$ [37] with P the polarization vector and N the charge density, Eq. (1) becomes:

$$\frac{d^2P}{dt^2}+\frac{q}{m\mu^{imag}}\frac{dP}{dt}+\frac{K_o}{m}P=\frac{Nq^2E}{m} \qquad (2)$$

We considered the solutions of Eq. (2) in the form $P = P_0e^{j[(\omega-\tau)t+\Phi]}$,
with ω the pulsation, Φ the phase difference between the polarization vector and the applied electric field, τ the parameter measuring the adiabatic evolution of the system.

By replacing P and $E = E_0e^{j(\omega-\tau)t}$ Eq. (2), we obtain:

$$\frac{P_0}{E_0}=\frac{Nq^2}{m}\frac{e^{-j\Phi}}{-(\omega-\tau)^2+jq\dfrac{(\omega-\tau)}{m\mu^{imag}}+\dfrac{K_0}{m}} \qquad (3)$$

Considering this organic polymer as a flat capacitor of surface A and distance separating the faces opposite L, its capacitance is given by:

$$\begin{aligned}C&=\mathrm{Re}\left(\frac{P_0A}{E_0L}\right)\\&=\mathrm{Re}\left(\frac{Nq^2A}{mL}\frac{e^{-j\Phi}}{-(\omega-\tau)^2+jq\dfrac{(\omega-\tau)}{m\mu^{imag}}+\dfrac{K_0}{m}}\right)\\&=\frac{Nq^2A}{mL}\frac{\cos\Phi}{\omega_0^2-\omega^2+2\omega\tau-\dfrac{q\omega}{m\mu_N}+\dfrac{q\tau}{m\mu_N}}\end{aligned} \qquad (4)$$

With $\omega_0^2=\frac{K_0}{m}$ and $\mu^{imag}=-j\mu_N$.

3. Result and Discussions

Frequency(rad/s)	C(F) Experiments dada [33]	Kwok's Model [34]	You-lin wu et al Model [37]	New model for this work
30	-6.66×10-10	-6.69×10-10	-6.66×10-10	-6.66×10-10
100	-2.30×10-10	-2.88×10-10	-2.40×10-10	-2.89×10-10
300	-6.50×10-11	-6.98×10-11	-6.97×10-11	-6.6×10-11
1000	-1.40×10-11	-1.42×10-11	-1.41×10-11	-1.40×10-11

Table 1. Comparison of the negative capacitance values of the different models with those experimental

(rad/s) ω	(rad/s) ω_0	(m^{-3}) N	(rad) Φ	(rad/s) τ	($m^2.V^{-1}.S^{-1}$) μ_N
30	2.30×10^{12}	4×10^{21}	1.871768582	0.1204633262	$-1.885967181\times10^{-12}$
100	2.30×10^{12}	3.50×10^{21}	2.291907017	0.6513094658	$-2.932455751\times10^{-12}$
300	2.30×10^{12}	3.02×10^{21}	1.584969128	3.281276546	$-1.191691980\times10^{-11}$
1000	2.30×10^{12}	2.49×10^{21}	1.645007382	0.5115340410	$-3.442721795\times10^{-13}$

Table 2. Material parameters used to obtain the capacitance values in Table 1.

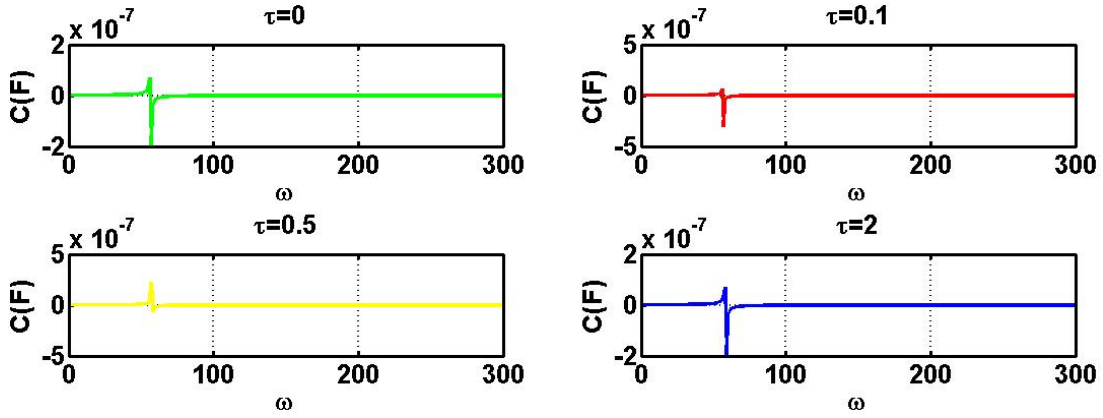

Figure 1. Simulated capacitance versus frequency curves when τ=0 rad/s, τ=0.1 rad/s, τ=0.5 rad/s, τ=2

Fig. 1 shows the curves giving the evolution of capacitance as a function of the frequency of the electric field and of the control parameter of the adiabatic evolution of the system. we find that at a certain frequency well determined, the attenuation of the vibration frequency of the polymeric materials by the parameter of the adiabatic evolution of the system τ increases the energy storage capacity of the given material. Between 0 and 50 rad/s, the capacitance remains constant and very close to 0 F, subsequently it varies in a positive and negative way before one again beginning its constant character.

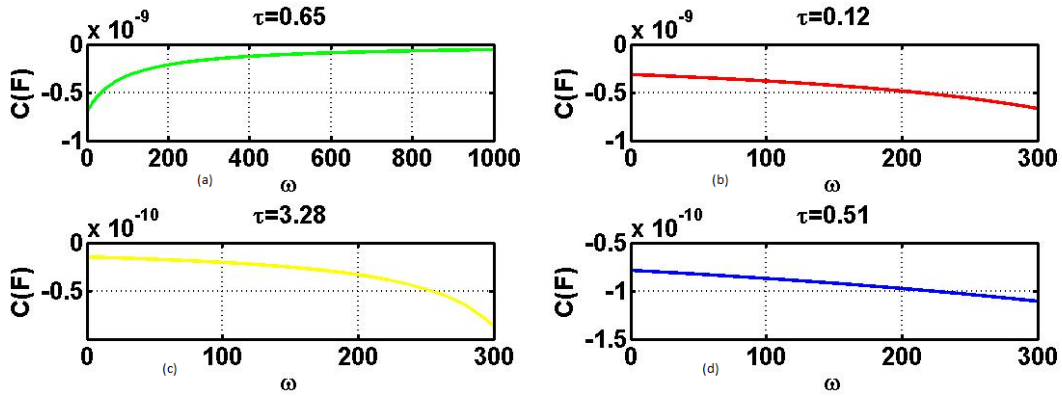

Figure 2. Capacitance versus frequency when : (a) τ=0.65 rad/s and Φ=2.29 rad , μ_N=$2.932455751\times10^{-12}$ $m^2.V^{-1}.S^{-1}$; (b) τ=0.12 rad/s and Φ=1.87 rad , μ_N=$-1.885967181\times10^{-11}$ $m^2.V^{-1}.S^{-1}$; (c) τ=3.28 rad/s and Φ =1.58 rad, μ_N=$-1.191691980\times10^{-11}$ $m^2.V^{-1}.S^{-1}$; (d) τ=0.51 rad/s and Φ=1.64 rad , μ_N= $-3.442721795\times10^{-13}$ $m^2.V^{-1}.S^{-1}$

Fig. 2 shows the evolution of the capacitance versus frequency for different value of Φ and μ_N.

We find that the capacitor made from polymer saturates at low frequencies, except for τ=0.65 rad/s where it saturates at high frequencies. values use to set the figures are contained in the previous tables to better highlight the negative character of the capacitance. higher the frequency of the external electric field is, greater the collisions between the charge carriers in the polymer and greater the effect of the potential wells that constitute traps for the movement of the particles, causing the movement of the charge carriers to be rather slow, so that the material will have a lower capacitance. τ is a function of the pulsation of the external disturbance which is the electric field here, indeed we can see that its value increases slowly with the pulsation of the field w. τ acts as a control parameter which can amplify or attenuate the frequency of charge carrier oscillation. There is an attenuation in our work.

The results we have obtained highlight the purely imaginary character of the electrical mobility of charge carriers in organic polymers, specifically poly p-phenylene vinylene. Indeed, starting from a new modified Paul Drude equation model proposed by us, translating the dynamics of holes in organic materials. Considering Eq. (2) and the values of the characteristic parameters of the organic polymer namely the charge density $N=10^{21}m^{-3}$, the mass m= $9.1\times1^{0-31}$kg, the thickness of the material $L= 2\times10^{-7}$m, the surface area A= 10^{-5} m^2, the charge q= 1.6×10^{-19}c [34].

4. Conclusions

In this paper, we have proposed a new equation model of the dynamics of electric charge carriers, more precisely that of holes. This new model is different from the two previous ones proposed by Kwok and You-Lin Wu in terms of electric mobility. Indeed, we introduce for the very first time the concept of pure imaginary mobility, associated to a control parameter of the adiabatic evolution of the system and to the phase difference between the mean position of the particle and the external perturbation. We are strongly convinced of the added value of this model, because thanks to it we have obtained experimental results on the existence of negative capacitance in poly p-phenylene vinylene.

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