SRCC

Scientific Reviews
&
Chemical Communications

Sci. Revs. Chem. Commun.: 2(3), 2012, 365-367
ISSN 2277-2669

CHARGE TRANSPORT IN HIGHLY CONDUCTING POLYMERS

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(*Received : 17.02.2012; Revised : 14.03.2012; Accepted : 23.03.2012*)

ABSTRACT

The theoretical ac conductivity $\sigma(\omega)$ of highly conducting polymer is studied. The composite medium is considered as metallic regions randomly distributed in the amorphous parts. Within the metallic regions, the polymer chains are regularly and densely packed, outside which the poorly arranged chains form amorphous host. The metallic grains are connected by resonance quantum tunneling, which occurs through the strongly localized states in the amorphous media.

Key words: Conducting polymers, AC Conductivity .

INTRODUCTION

The discovery of doped polyacety-lene in 1977[1], led to considerable interest in fundamental and applied research of highly conducting polymers such as doped polyacetylene, polyaniline, and polypyrrole. Attention is focused on the mobile charged defects (solitons, polarons, and bipolarons) in lightly doped one-dimensional chains and the disorder-induced charge localization in highly doped systems. The nature of the metallic state and the metal–insulator transition (MIT) in highly conducting polymers remain controversial and are not fully understood. The complex morphology of the materials originating from structure inhomogeneities in the nanolength scale is the cause of the complicated charge transport properties of highly conducting polymers.

X-ray-diffraction patterns of these materials show both crystalline and amorphous regions. The “metallic” polymers can therefore be described as disordered metal near the metal–insulator transition. The metallic states of highly doped conducting polymers are based upon both the nature of the metallic states of ordered regions and the charge transport properties in disordered regions.

Dc conductivity only is not sufficient to determine the charge transport mechanism in these materials. Romijn et al. studyied the polypyrrole samples in metallic and critical regime of metal–insulator transition (MIT)[2]. According to them both the coherent and incoherent transport (hopping) account for the ac

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*Author for correspondence; E-mail: rsbobade29@gmail.com conductivity in the highly conducting polymers. However, there is still a little theoretical work devoted to charge transport of these metallic polymers.

EXPERIMENTAL

Theory

Chain structure is of great importance in explanation of the charge transport in highly conducting polymers. Structure study[3,4] shows that there are crystalline regions where the polymer chains are regularly and densely packed. The electron wave function is extended over the whole domain volume, therefore the crystalline regions can be considered as metallic grains. Drude type metallic behavior has been demonstrated in these three-dimensional and highly conducting regions, and in the form of the standard Drude formula –

$$\sigma_{(\mathrm{Drude})}(\omega) = \frac{1}{4\pi}\,\frac{1\omega_{p}^{2}\,\tau_{1}}{1-i\,\omega\,\tau_{1}} \qquad \ldots(1)$$

with ω_p being "the plasma frequency" and τ_1 the low frequency relaxation time. $\tau_1 \sim 10^{-12}$ s and $\omega p \sim 1/\tau_1$, which are experimentally identified [5,6]. Outside these regions, however, the order in chain arrangement is poor. The electronic states of amorphous chains are strongly localized and chains are non interacting in this region. These polymer chains therefore form amorphous media with localized states. The conductivity here proves purely capacitive and can be written as –

$$\sigma(\omega) = -i\omega e^{2} c\, \mathrm{N}\,(\varepsilon_F)\, R^{2} \qquad \ldots(2)$$

where e is the electric charge, c is the degree of crystallinity and R the related size of grain. $N(\varepsilon_F)$ is density of states per unit cell. These metallic islands are coupled into a granular network with the twisted polymer chains. Thus we come to the model of a granular metal of nanoscale metallic dots embedded in amorphous poorly conducting medium for description of transport in the highly conducting polymers.

In the structure of highly conducting polymers the regions where the polymer chains are regularly and densely packed correspond to crystalline regions. The amorphous regions demonstrate poor chain order. Therefore the system is modeled as a composite medium consisting of metallic regions randomly distributed in the amorphous parts. Note that the polymer grain has essentially quantum size and the shape of grains cannot be described by a simple geometry form. Unlike the standard metal, where the electric coupling is based on mechanic contacts, the metallic dots in polymers are spatially separated by amorphous regions and the coupling is provided by single polymer chains. The transmission coefficient g for direct tunneling is about 10^{-4}, essentially suppressed[7]. The intergrain tunneling occurs mostly through the localized states in the disordered parts with strong contribution from resonant states whose energy is close to the Fermi level. And the intergrain transmission coefficient is equal to 1 for resonance tunneling. For the highly conducting polymers, there are about 100 polymer chains connecting one grains with the other, this resonant tunneling dominates the entire charge transport through a grain though the coupling occurs only through single resonant chains out of the whole bundle of chains connecting the metallic grains. For resonance tunneling the frequency dependent transmission coefficient $g = g(\omega)$ is given by generalization of Bright–Wigner formula[8,9].

$$\mathrm{gBW}\,(\omega) = \left[1-\frac{i\,\omega}{\gamma}\right]^{-1} \qquad \ldots(3)$$

where γ is the width of the resonance level and $\gamma = (1/\tau)\exp(-L/\xi)$.

For samples of 50% crystallinity, L is of the same order as a grain size R. ξ is the localization length and is about 1 nm. τ is the scattering time and can be calculated from optical measurements and is about 10^{-15} s[10]. It is assumed that if two metallic regions are not far away from each other, they are always coupled into network with tangled polymer chains. The above considerations help to consider the ac conductivity $\sigma(\omega)$ of highly conducting polymer. A heterogeneous model, in which the metallic region is modeled as a Drude conductor while the amorphous region as a parallel combination of a resistor and a capacitor, can also fit this well.

CONCLUSION

The ac conductivity $\sigma(\omega)$ explains the charge transport of highly conducting polymer . Taking into account the complicated morphology of the highly doped conducting polymers, i.e., both the properties of the metallic states in the ordered regions and the charge transport properties in disordered regions, we model the system as a composite medium consisting of metallic grains randomly distributed in the amorphous parts. In the metallic regions, the polymer chains are regularly and densely packed, while outside which the poorly arranged chains form amorphous host. The metallic grains are connected by resonance quantum tunneling, which occurs through the strongly localized states in the amorphous media.

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