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Theoretical approach of the electroluminescence quenching in (polymer-CdSe quantum dot) nanocomposite

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ABSTRACT

A theoretical approach based on the rate equation of exciton density for the electroluminescence quenching in (polymers-quantum dots) nanocomposite is developed. It is shown that the light intensity observed in the nanocomposite depends respectively on the quantum dots concentration, the injected charge carriers, the exciton density, and the Förster energy transfer between polymer and quantum dots. We have found that the significant reduction of the light intensity is related to the exciton density profiles which exhibit a monotonic decrease with the increase of Förster transfer mechanism. Our theoretical approach for the electroluminescence agrees with experimental results observed in hybrid structure (MEH-PPV) with CdSe quantum dots. The maximum of exciton density is also estimated and we have obtained a value for the exciton diffusion length of 10 nm which is consistent with the available experimental results.

1. Introduction

In recent years, the incorporation of inorganic II-VI semiconductors quantum dots (Qds) such as ZnSe, ZnS, ZnO, CdS and CdSe into polymer matrix has been offered special interest for both

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experimental and theoretical considerations [1–7]. This is due to the fact that these nanocomposite materials are extensively used in optoelectronic devices such as photovoltaic solar cells and light emitting diodes (LEDs) [8–11]. It is well known that the incorporation of Qds in polymer is expected to increase brightness and to enhance the performance of the device [12–14]. For example, in our previous work [15], we have investigated the effect of ZnSe quantum dot concentration on the fluorescence enhancement of polymer P3HT film. Zou et al. [16] have also reported the emission enhancement of polyfluorene doped with ZnO nanoparticles. Unfortunately, the incorporation of the Qds with polymer can also play an opposite role, it can caused a considerably reduction for the emission. This reduction has been reported in the majority of experimental works performed on the nanocomposite that contains especially CdSe Qds [17–20]. An interesting question has been related to the concentration of CdSe Qds that will be added to the polymers matrix. J.H. Park et al. [21] have reported on the performance of electroluminescence (EL) of polymer-CdSe double-layer LEDs. The authors showed that there are negative effects of using CdSe nanoparticles in EL devices especially for high concentration of CdSe and in the case of low concentration the light intensity of nanocomposite is not quenched rather it is increased. In other work [22,23] the authors suggested that CdSe Qds improved significantly the emission of the devices only for a non-uniform dispersion of Qds in the polymer layer. Recently [24], a significant quenching of light emission has been observed with increased CdSe Qds concentration in (MEH–PPV). More recently [25,26], a significant reduction of the light intensity with increased Qds concentration has been observed. However, we believe that these important experimental works need a theoretical approach to explain some results. In this study, we would like to develop a theoretical model to describe the Qds concentration, the exciton density profiles and the EL intensity in the device. We have chosen the hybrid structure such as (MEH-PPV-CdSe) as an example. This theoretical model is based essentially on four physical processes: the transport and diffusion of the charge carrier in the nanocomposite, the exciton creation, the Förster energy transfer between polymer and Qds and finally the light emission in the hybrid material. In particular, the exciton density profiles in the emissive layer of the nanocomposite are performed for different parameters such as the concentration of injected charge carriers, the Qds capping thickness layer and the Förster transfer rate. Finally, we believe that one of the key design aspects of (Qds-LED) performance can be associated to the optimal concentration of Qds which lead to high light emission intensity.

2. Theoretical approach and numerical resolution

The method used to study the El intensity in hybrid organic–inorganic material is based on the rate equation model taking into account the optimization of the Qds concentration, the injected charge carriers density, the Qds shell thickness and the distance x from the electrodes where exciton density is maximal.

2.1. Charge injection from an electrode and charge carrier transport

It is well known that in the El process the holes and electrons are injected in the nanocomposite respectively from anode with high function work and cathode with low function work. In this work, we have used (CdSe Qds embedded in a MEH-PPV layer) as an hybrid material and (ITO) as anode and (Al) as cathode. The polymer (MEH-PPV) is considered as one of the most popular polymer for hybrid electroluminescent devices [21,24]. The band structure of (MEH-PPV) with CdSe Qds presented in Fig. 1 shows that these nanocomposites are favorable for charge transport. In order to control the dispersion and concentration of CdSe Qds in the organic layer, we assume that the transport of carrier charge can be described by both drift and diffusion currents. The diffusion phenomena can be privileged for organic system because that the polymer structures have a larger disorder in which transport can be described in terms of hopping between strongly localized states [27,28]; while the drift current becomes important only for a large applied electric field ($E \geqslant 10^5$ V cm^{-1}) [29]. The current densities for electrons and holes can be expressed as the sum of drift and diffusion currents: