

L.9: Charge transport in polymer nano-composite thin films for photovoltaic applications

Polymer nanocomposites are promising photoactive materials for the development of cost effective photovoltaic cells. The desired properties of polymer materials for photovoltaic applications are efficient charge generation and higher mobility of photoinduced free charge carriers. To meet these requirements, polymer nanocomposite films are fabricated by dispersing semiconducting polymers with nanoparticles of suitable inorganic semiconductors. We made systematic studies on the observed enhancement of hole mobility with increasing concentration of nanoparticles and also discuss the possible mechanism of mobility enhancement. Our investigations were on thin films of Poly(2-methoxy-5-(3',7'-dimethyloctyloxy)-1,4-phenylenevinylene) (MDMO PPV) polymer dispersed with lead sulphide (PbS) nanoparticles (MDMO PPV:PbS). Mobility was obtained using transient photoconductivity experiment. Increase in mobility with nanoparticle concentrations was attributed to increase in polymer inter-chain interaction and also to the tunneling of carriers through nanoparticles.

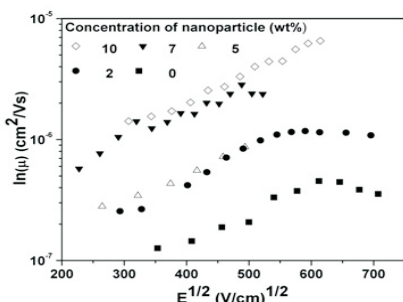


Fig. L.9.1: Field dependence of mobility in MDMO PPV:PbS at various concentrations of nanoparticles.

In all MDMO PPV:PbS thin films, carrier mobility increases with applied electric field strength (Figure L.9.1). Increase in mobility with electric field is due to the decrease in the energetic barrier, which carrier encounters while hopping, by the applied electric field. Compared to pristine MDMO PPV, mobility is enhanced by an order upon dispersing nanoparticles.

Dispersing the nanoparticles in the polymer matrix can change the polymer film morphology, which can remarkably influence the charge carrier hopping rate and subsequently the mobility. To gain insight into the changes in the polymer film morphology due to PbS nanoparticles, we made photoluminescence (PL) and Raman measurements. PL of polymer in MDMO PPV:PbS thin films with various PbS concentrations is shown in Figure L.9.2. Three main PL peaks observed at ~590 nm, ~640 nm and ~700 nm are assigned to be the 0-0, 0-1 and 0-2 transitions respectively.

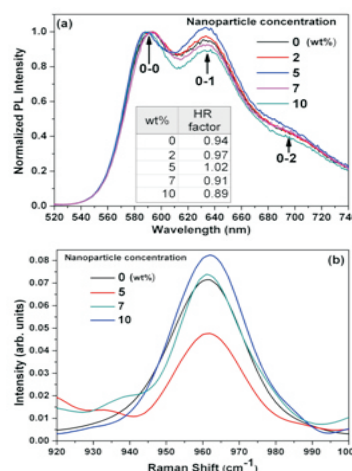


Fig. L.9.2: (a) PL spectra (b) Variation in the intensity of ~963 cm⁻¹ Raman mode of MDMO PPV:PbS thin films at various PbS concentrations.

Significant changes are observed in the relative intensity of 0-0 and 0-1 transitions upon increasing the PbS concentration. This infers the changes in the electron phonon coupling factor (Huang Rhys (HR) factor) between the polymer chains, i.e. variation in polymer inter-chain interaction with nanoparticle concentration. Higher the HR factor stronger is the polymer inter-chain interaction and vice versa. HR factor increases with PbS concentration and attains a maximum value at ~5 wt%. HR factor decreases at higher PbS concentration (7 wt% & 10 wt%). Hence, PL studies show enhancement in polymer inter-chain interaction up to 5 wt% of PbS concentration beyond which inter-chain interaction decreases.

Changes in the Raman mode related to the out of plane C-H wagging of the vinylene group (~963 cm⁻¹) of MDMO PPV is shown in Figure L.9.2. Decrease in the intensity of ~963 cm⁻¹ mode at low PbS concentration suggests that out of plane wagging get restricted, i.e. polymer chains get tightly packed. At concentration beyond 5 wt% the intensity of ~963 cm⁻¹ mode increases, which suggests that polymer chains are getting loosely packed. Tighter the polymer chain packing stronger is the polymer inter-chain interaction and vice versa.

Thus, at low PbS concentration the increase in the inter-chain interaction and the tunneling of carriers through nanoparticles is responsible for the enhancement in carrier mobility. At higher PbS concentrations, the increase in mobility even when there is a decrease of inter-chain interaction suggests that the mobility enhancement can be attributed only to tunneling of carriers through nanoparticles. For more details refer: Synth. Met. 224, 80, 2017, J. Polym. Sci. Part B: Polym. Phys., 53, 1431, 2015.

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