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Studies on Structure and Raman spectroscopy of Ni-doped copper phthalocyanine thin films

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Abstract

Ni-doped copper phthalocyanine (CuPc) organic films with different mixing ratios were prepared in high vacuum (HV) chamber. The results of AFM, XRD, UV-vis and Raman spectroscopy indicated that the surface morphologies of the films were found to be flatter and the structures of the CuPc films still kept their original α -phase crystal, with only the crystallinity or crystallite sizes being changed and the versatile structure or charge transport being modified with the increase of Ni-doping ratios. Moreover, 514nm-visible-light-excited normal Raman spectra (NRS), 325nm-ultraviolet-excited and 633nm-excited resonance Raman spectra (RRS) were analyzed by comparison and by density functional theory (DFT) calculations of the amorphous nickel atoms clusters, confirming that there were no chemical changes between CuPc molecules and nickel atoms; and the amorphous nickel atoms clusters had a noticeable light absorption loss, offering us an insightful structural understanding of the Raman effect of the different concentrations of Ni-doped CuPc films.

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Keywords: Organic thin film; the amorphous nickel atoms clusters; Raman polarization; resonance Raman spectra; Ni-Doped.

1. Introduction

There has been increasing interest in organic semiconductor thin films (OSTF's) because of their potentially useful optical, electrical and magnetic properties in optoelectronic devices and organic semiconductor devices, and so on [1,2]. Recently, the use of transition metal nanoparticles embedded in organic semiconductors appears to be one of the promising applications. Reports can also be found in which transition metal nanoparticles were used as dopants to enhance the quantum efficiency of an organic light emitting device (OLED) [3] or to provide a large magneto-resistance in organic-based spin device, see e.g. Co nanoparticles in rubrene [4] or fullerene [5] matrices.

The deposition of organic thin film and metal-organic multilayer thin film in HV chamber became a main technological method for organic micro- and nano-device technologies [6–8]. All these new technologies have the need for modulation of the photoelectric properties of OSTF's for these upcoming devices. Phthalocyanine materials are well known for their semiconducting behaviour and possess promising optical and electrical properties [9]. As an organic semiconductor material, CuPc shows sufficient chemical and thermal stability to allow purification by sublimation techniques at a necessarily high temperature and vapor deposition [10]. These films then possess excellent and well defined electronic or optoelectronic properties [11,12]. CuPc is a semiconducting molecular crystal having several polymorphic forms which determine the energy state, the band gap and the anisotropy of electrical conductivity; among various polymorphs, the α and β ones are the best known and the most widely studied.

As a ferromagnetic metal, nickel (Ni) attracts extensive studies and is used in various applications. To the best of our knowledge, the Ni-doped CuPc organic film has never been studied in a deep-going way. In the case of the mixed film, the knowledge of the surface morphology and the preferred orientation of the crystallites are essential for their successful applications [13]. In spite of their remarkable properties of metal-doped OSTF's in general, there is no complete understanding of this class of films [14]. For the intended future applications of these materials it is necessary to have a precise knowledge of the interaction and crystallization mechanisms on substrates and a practical experience of how to achieve certain parts of an apparatus or appliance.

Thus this work focuses on the determination of structural, morphological and photoelectric properties of Ni-doped CuPc organic films. AFM, X-ray diffraction, UV-vis and Raman spectroscopy have been studied, the results indicated that the surface morphologies of the films were found to be flatter, the crystallinity or crystallite sizes were changed and the versatile structural or charge transport

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