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Enhancing charge transport in copper phthalocyanine thin film by elevating pressure of deposition chamber



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ABSTRACT

Copper phthalocyanine (CuPc)-based thin film transistors were fabricated using CuPc films grown under different deposition pressure ($P_{\rm dep}$) (ranging from 1.8×10^{-4} Pa to 1.0×10^{-1} Pa). The transistor performance highly depended on $P_{\rm dep}$. A field-effect mobility of 2.1×10^{-2} cm²/(V s) was achieved under 1.0×10^{-1} Pa. Detailed investigations revealed that $P_{\rm dep}$ modulates the molecular packing and orientation of the organic films grown on a SiO₂/Si substrate and influences the charge transport. Furthermore, from a device physics point of view, contact resistance of the fabricated transistors decreased when $P_{\rm dep}$ increased, which was beneficial in reducing energy consumption.

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1. Introduction

Organic thin film transistors (OTFTs) have been the subject of intensive interest because of their applications in low-cost and large-area electronics [1,2]. Great efforts have been devoted to the improvement of device performance, which still remains one of the most critical issues in developing OTFTs. Generally, the optimization of molecular packing in the crystalline phase of organic semiconductors may facilitate charge hopping among the molecules, leading to the enhancement in electrical characteristics of OTFTs [3–6]. In the fabrication of OTFTs through vacuum deposition, the molecular packing in active thin films is usually optimized by regulating the temperature and surface properties of the substrate, since the weak van der Waals force among the organic molecules can be easily disturbed during the self-assembly process [7–10].

Recently, we observed that increasing deposition pressure $(P_{\rm dep})$ modulated the orientation tendency of the deposited copper phthalocyanine (CuPc) molecules to be more perpendicular to the substrate, and the device performance of OTFTs was effectively enhanced [11]. However, the intrinsic correlation between the thin-film microstructure and the corresponding device performance is still lacking, to understand the relationship between these two phenomena is of great interest and significant importance for the improvement of device performance.

For organic semiconductors, it has been well documented that charge transfer between adjacent molecules can use a thermally activated hopping mechanism. Mobility obeys Arrhenius-type dependences [12]:

$$\mu = \mu_0 \exp\left(\frac{-E_{\rm a}}{kT}\right),\tag{1}$$

where k is the Boltzmann constant, T is the temperature, μ_0 is the prefactor and $E_{\rm a}$ is the activation energy. Combined with the Meyer–Neldel rule and the Gaussian

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disorder model, the activation energy E_a can be described as [13]:

$$E_a = \left\lceil 0.75 - 0.67 \log_{10} \left(\frac{n}{N}\right) \right\rceil \sigma, \tag{2} \label{eq:eaction}$$

where n/N is the relative carrier concentration, and σ is the Gaussian density of states (DOS). For the same gate voltage, $V_{\rm g}$, which means for the same effective n/N. Due to the different σ the $E_{\rm a}$ are different. So σ can be used as an important material characterizing parameter for active organic semiconductor layers in OTFTs independent of the device geometry [14]. Moreover, in the perspective of the quantum-chemical calculations, charge transfer among molecules can be described by the Marcus theory [15,16].

Here, we thermally deposited CuPc in vacuum onto the SiO₂/Si substrates at different $P_{\rm dep}$. Electrical performances of the fabricated OTFTs significantly improved when $P_{\rm dep}$ was increased, exhibiting a field-effect mobility ($\mu_{\rm FET}$) of $2.0\times 10^{-2}~{\rm cm}^2/({\rm V~s})$ and an on/off ratio greater than 10^5 . Investigations on the crystalline property of deposited CuPc films revealed that the molecular packing was modulated when $P_{\rm dep}$ was increased. Therefore, the activation energy required for the charge hopping between adjacent molecules was reduced, and charge transport in the active layer was enhanced. Furthermore, the Y function method clearly indicated that contact resistance ($R_{\rm C}$) was lowered when $P_{\rm dep}$ was increased.

2. Experimental

The CuPc with 99% purity was purchased from Aldrich and used without further purification. Fig. 1a illustrates the schematic structure of CuPc-based OTFTs, which is fabricated in the similar way to our recent report [11]. A heavilv doped n-type (100) Si substrate with a 300 nm SiO₂ layer was cleaned in an ultrasonic bath successively using acetone, isopropyl alcohol, and deionized water. The substrates were placed in the chamber and maintained at 5×10^{-5} Pa for 4 h. And then, the chamber pressure was adjusted by injecting high-purity nitrogen to be under a specific deposition pressure (P_{dep} , i.e., 10^{-4} , 10^{-3} , 10^{-2} , and 10^{-1} Pa). The deposition rate for CuPc was kept as low as 0.08 Å/s, and the substrate temperature was maintained at 125 °C during deposition. The thickness of resulting CuPc films were approximately 50 nm. Finally, a 50 nm Au electrodes were thermally deposited through a shadow mask. Therefore, the CuPc-based OTFTs had a bottom-gate top-contact architecture with the channel length (L) and width (W) of 50 and 500 μ m, respectively.

The surface morphology and crystalline structure of the CuPc film were characterized by scanning electron microscopy (SEM, Hitachi S-4800, operating at 3 kV) and X-ray diffraction (XRD, Panalytical X'pert Pro X-ray diffractometer, Cu target, operating at 40 kV and 40 mA, $K_{\alpha 1}$ = 1.54056 Å). The measurement of transistor characteristics was performed using a Keithley 4200-SCS semiconductor parameter analyzer. The measurements of the $I_{\rm d}$ – $V_{\rm g}$ characteristics in the linear regime (at source–drain

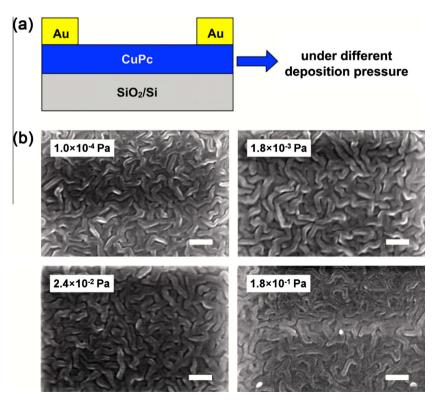


Fig. 1. (a) Schematic structure of CuPc-based OTFTs. (b) Scanning electron microscopy images of 50 nm CuPc films deposited on SiO_2 at a substrate temperature of 125 °C under different P_{dep} values. All scale bars correspond to 200 nm.

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