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Characterization of titanyl phthalocyanine (TiOPc) thin films by microscopic and spectroscopic method

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ABSTRACT

The titanyl phthalocyanine (TiOPc) thin film deposited on glass, silicon and gold substrate have been studied using Raman spectroscopy, atomic force microscopy (AFM), absorption and profilometry measurements. The TiOPc thin layers have been deposited at room temperature by the quasi-molecular beam evaporation technique. The Raman spectra have been recorded using micro Raman system equipped with a confocal microscope. Using surface Raman mapping techni que with polarized Raman spectra the polymorphic forms of the TiOPc thin films distribution have been obtained. The AFM height and phase image were examined in order to find surface features and morphology of the thin films. Additionally to compare experimental results, structure optimization and vibrational spectra calculation of single TiOPc molecule were performed using DFT calculations. The received results showed that the parameters like polymorphic form, grain size, roughness of the surface in TiOPc thin films can well characterize the obtained organic thin films structures in terms of their use in optoelectronics and photovoltaics devices.

1. Introduction

Organic thin film structures based on metallophthalocyanine molecules possess very interesting optical and electrical properties. This type structures obtained by various deposition techniques on solid state substrates have become widely used materials. An important feature of these materials is the low cost of production and the receipt of structures with very stable chemical and thermal parameters. Especially in the form of thin films, can be applicable in many advanced technological devices [1–3]. Thin layers of metallophthalocyanines (MPc) as well as their junctions with a number of organic and inorganic semiconductors or metals can be applicable in optoelectronic as for example light-emitting diodes, photovoltaic cells, and organic field effect transistors construction [4,5]. For this reason the knowledge of their molecular orientation, surface morphology of thin layers and thus optical and electrical properties is very important.

Metallophthalocyanines can occur in many polymorphic phases α, β, χ, and ε connected with different crystalline structure. The most popular is metastable α form and stable β form. The main difference between both forms is the tilt angle of the molecule within the columns and arrangement of the common columns in the crystalline structure. These parameters play a significant role in changes of conductivity along stacking molecules. Notably, chemical nature of the metallophthalocyanine, as well as substrate's geometry and temperature play a very important role. The influence of the substrate of that kind and its temperature on the growth of MPc layers still is not well recognized and understood [6,7,11,19].

Thin films of metallophthalocyanine have been recently intensively investigated by many experimental method such as especially as absorption, ellipsometry, harmonic generation, AFM imaging and Raman spectroscopy [6–11]. The Raman spectroscopy can be useful tool to study of various intra- and intermolecular energy transfer processes.

In case of TiOPc thin films, the knowledge of the surface morphology and the preferred orientation of the crystallites and their electrical parameters are essential for potential successful applications. The preferred orientation is usually determined by sample preparation conditions for example such as type of substrate and method of evaporation.

In this paper we will present the results of the research on the structural orientation of TiOPc thin films deposited on silicon substrate using

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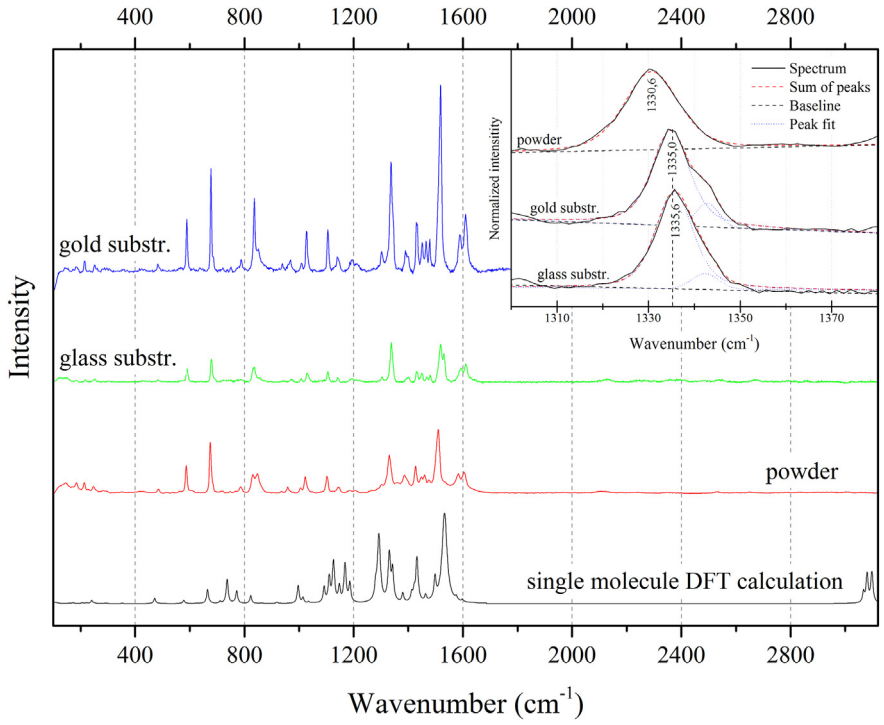

Fig. 1. Comparison of Raman spectra of TiOPc powder, thin films on gold and glass substrate and calculated Raman spectrum.

microscopic method such as atomic force microscopy (AFM) and Raman microscopy. Additionally, using quantum mechanical calculations, we received important information about the structure of the molecule and its normal vibrations. The use of computational techniques supports the experiment and is a useful tool for the correct interpretation of the results of the Raman light scattering experiment.

2. Experimental

2.1. Preparation of the Thin Films

The titanyl phthalocyanine (TiOPc) thin films were prepared by deposition at room temperature by the molecular beam deposition

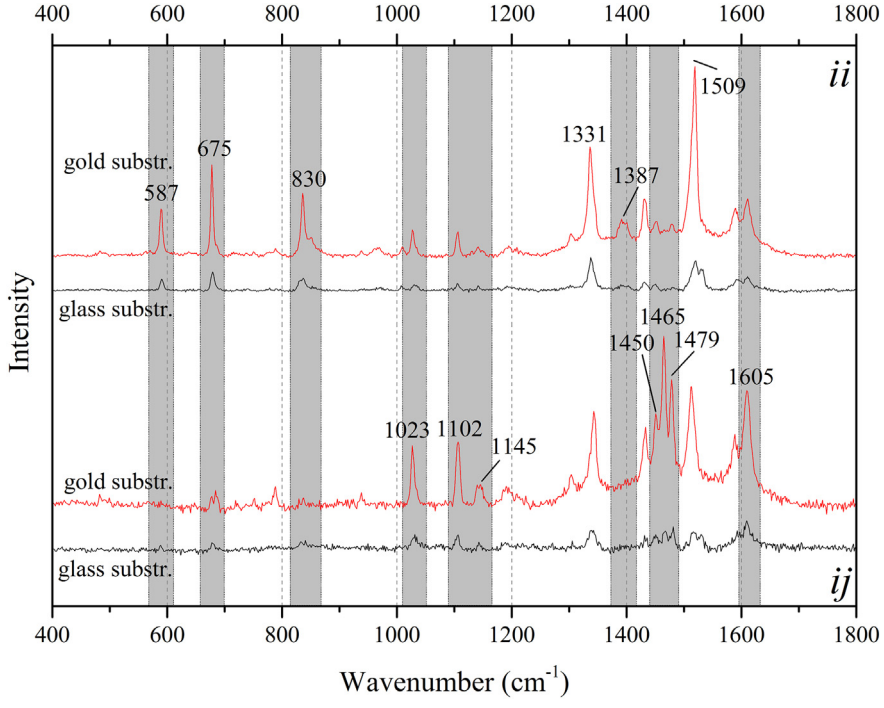

Fig. 2. Comparison of polarized Raman spectra of TiOPc thin film on gold and glass substrate.