

MS43-P8 Efficient sensing of explosives by using highly textured fluorescent nonporous films of oligophenyleneethynylene derivatives

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The fluorescence of thin films of diimine-substituted phenyleneethynylene can be efficiently quenched by nitroaromatic vapors, which is not the case for the unsubstituted parent compound. Thin film porosity is usually considered to be an essential factor for efficient quenching, but in the present case the origin is completely different, as both films are non-porous and hermetic to DNT/TNT molecules. The explanation for this very efficient sensing comes from the molecular organization in the two crystallized thin films. By combining the information from single-crystal and thin film diffraction experiments it is shown that π -stacking in the structure of both the substituted and the non-substituted compound is not very pronounced, but that the orientation of the phenyleneethynylene fluorophore differs markedly with respect to the surface of the film. For the substituted compound, the fluorophore is almost parallel to the surface, thus making it readily available to molecules of a nitroaromatic quencher. This rationale is also observed in the case of a related compound bearing methoxy side chains instead of the long octyloxy moieties. Fluorescence lifetime experiments show that the efficient quenching process in the non-porous, crystallized films of the substituted compound is due to a fast (<70ps) diffusion of excitons from the bulk of the film toward its surface where they are quenched.

Keywords: thin films, explosives, diffraction, fluorescence

MS43-P9 Cathodic arc evaporation of oxide coatings: investigation of the phase transformation at the target surface and deposition of Al and Hf oxides

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Reactive cathodic arc evaporation is an attractive method to produce oxide coatings for a wide variety of applications, e.g. for oxidation and chemical protective coatings, diffusion barriers, or for wear protection in tribological systems [1]. One reason for this is the possibility to control the phases and phase compositions of the synthesized oxides by the chemical composition of compound targets utilized as cathodes for the evaporation. The oxygen flow influences the evaporation rates of the cathode material as well as the conditions under which the metallic vapour condenses and reacts at the substrate surface. To control these parameters, it is necessary to understand the process related to the oxide synthesis. We are therefore active in studying the phase transformation at the target (cathode) surface after the arc process and to correlate the results with the phases obtained in the coating [2]. The example of the Al-Hf system is given in Fig. 1.

The targets were operated with and without oxygen reactive gas. The phase composition at the target surface was determined by X-ray diffraction (XRD) analyses and compared for the different process conditions. Coatings were deposited for each process parameter set utilized for surface treatment of the targets. The compositions of the layers were determined by Rutherford backscattering spectrometry. XRD was used to determine the metallic and oxide phases in the layers. A comparison of the phase composition between layers and target surface is given and the possible processes during target surface modifications are discussed. In addition, high temperature in-situ XRD measurements up to 1290°C were performed to study the process of oxide formation from intermetallic compounds in the layers [2]. As a result, the oxide coatings produced by this state-of the art reactive cathodic arc evaporation process are well suited for applications in high temperature environment, especially as oxidation and diffusion barriers.

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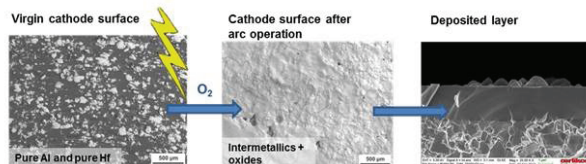


Figure 1. SEM images of a composite Al-Hf cathode surface before (left) and after the arc operation (middle) and the associated deposited layer (right).

Keywords: in-situ XRD, hard coatings, intermetallics, target processes, layers

MS43-P10 Thin film polymorphism in organic semiconductors

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Polymorphism is a phenomenon which is crucial to the understanding of crystal nucleation and growth, and establishment of structure–property correlation.¹ It is a phenomenon with high industrial significance particularly in pharmaceutical industry. Given the importance of polymorphism in determining the property of materials, a topic of recent interest is to study how it affects the performance of functional materials in the field of organic electronics. Although, presence of several polymorphic forms facilitates the study of charge-transport behaviour with respect to crystal packing, it may hinder the reproducibility, reliability, and stability of the devices fabricated using such materials. Research is being carried out to identify specific polymorphic phases of organic thin films, where the polymorphism exists near the substrate.² Depending on film thickness, deposition methodologies, temperature etc, a particular phase may exist. Under certain circumstances it may be possible to induce transformation from one phase to another. The physical and chemical factors that drive such a process are not yet clearly understood. Hence, it is of utmost importance to identify the phases and to control the formation of the different forms. In particular, this is really crucial in the field of organic electronics, where the charge-transport properties are highly dependent on crystal packing, especially for organic field-effect transistors where charge transport occurs at the interface between the organic semiconductor and the dielectric. In this presentation, we present an overview of the recent advances done in our group in this topic. Especially, [1]benzothieno[3,2-b][1]benzothiophene (**BTBT**) based semiconductors which are gradually emerging as the most promising organic semiconductor are the principal objects of our study. Structural and morphological studies of library of BTBT-based compounds are presented to gain more insights into the phenomenon.

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Keywords: Polymorphism, Thin Films, X-ray diffraction,