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Division of Multidisciplinary Chemistry
- Molecular Aggregation Analysis -

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Prof BOUVET, Marcel — Ecole Supérieure de Physique et Chimie Industrielles de la ville de Paris, France, 4–17 November 2007

Scope of Research

The research at this subdivision is devoted to correlation studies on structures and properties of both natural and artificial molecular aggregates from two main standpoints: photoelectric and dielectric properties. The electronic structure of organic thin films is studied using photoemission and inverse photoemission spectrosocpies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous sturcutres in microcapsules, biopolymers, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

Research Activities (Year 2007)

Publication

Yoshida H, Inaba K, Sato N: X-ray Diffraction Reciprocal Space Mapping Study of the Thin Film Phase of Pentacene, *Appl. Phys. Lett.*, **90**, 181930 (2007).

Presentations

Direct Observation of Electron and Hole Transport Levels in Organic Thin Films (in Japanese), Sato N, Research Meeting "Organic Electroluminescent Devices – New Developments from Now On" of Division of Molecular Electronics and Bioelectronics, The Japan Society of Applied Physics (Uji, Japan), 6 March 2007.

Dielectric Spectra of Biological Cell and Tissues Simulated by Three-dimensional Finite Difference Method, Asami K, The 13th International Conference on Electrical Bioimpedance Combined with the 8th Conference on Electrical Impedance Tomography (Graz, Austria) 29 August–2 September 2007.

Structures and Surface Electronic Properties of Evaporated Thin Films of a Series of Zwitterionic Molecules, Tsutsumi J, Yoshida H, Sato N, Kato S, The 4th Workshop on Advanced Spectroscopy of Organic Materials for Electronic Applications (Chiba, Japan), 8–12 October 2007.

The Crystallographic and Electronic Structures of Three Different Polymorphs of Pentacene, Yoshida H, Sato N, The 9th China-Japan Joint Symposium on Conduction and Photo-conduction in Organic Solids and Related Phenomena (Beijing, China), 27–29 October 2007.

Grants

Sato N, Development of Novel Electronic Systems Based on Hybridization of Characteristic Molecular

X-ray Diffraction Reciprocal Space Mapping Study of the Thin Film Phase of Pentacene

Pentacene thin films are extensively studied in connection with their application to organic field-effect transistors. To understand transport properties in those films, precise information on their structure is indispensable. On the other hand, pentacene thin films are known to show a few polymorphs usually distinguished by the interlayer spacing along the c^*-axis. Among them only the polymorph of "single crystal" phase (d_{001} = 1.41 nm) has so far disclosed the complete crystallographic data.

The "thin film" phase (d_{001} = 1.54 nm) is observed for a film in the thickness less than 100 nm vacuum-deposited on an insulating layer such as SiO_2; the structural information of this phase is particularly relevant, since this polymorph is often realized in the working layer in pentacene thin-film field effect transistors. Previous structural studies on this phase have been carried out using electron diffraction, grazing incidence X-ray diffraction (GIXD) as well as the θ-2θ scan of X-ray diffraction. The structural data obtained from these methods, however, are not enough to determine even the crystal system of the phase between monoclinic and triclinic ones. In this work we employed X-ray diffraction reciprocal space mapping (RSM) method to analyze the crystallographic structure of the thin film phase of pentacene. The obtained structure in comparison with that of the bulk phase is shown in Figure 1 and can be applied to the energy band calculation.

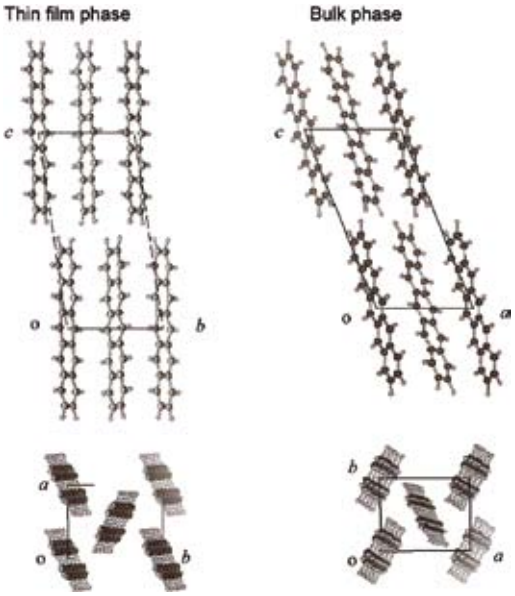

Figure 1. Structures of the thin-film and bulk phases of pentacene.

Dielectric Properties of Water in Triton X-100 (Nonionic Detergent) – Water Mixtures

Dielectric measurements were carried out for mixtures of Triton X-100 (TX, a nonionic detergent with a poly(ethylene oxide) chain) and water with or without electrolytes over a frequency range of 1 MHz to 10 GHz to study the structure and dynamics of water molecules in the mixtures (Figure 2). Dielectric relaxation was found above 100 MHz, being assigned to the dielectric relaxation of water. The intensity of the dielectric relaxation was proportional to the water content above 0 °C. Below the freezing temperature of bulk water, the relaxation intensity decreased at TX concentrations (C_{TX}) below 50 wt% at –10 °C and below 60 wt% at –20 °C because frozen water shifts the dielectric relaxation to a frequency region far below 1 MHz. This indicated that there is no bulk water at C_{TX} above 50 wt% and that at least two water molecules per ethylene oxide (EO) unit are tightly associated with the ethylene oxide chain. The low-frequency conductivity of the mixtures of TX and electrolyte solutions was well represented by Bruggeman's mixture equation at C_{TX} below 40 wt%, if two water molecules per EO unit form an insulating shell surrounding TX micelles.

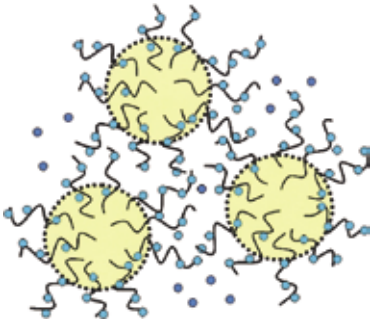

Figure 2. Schematic representation of TX micelles whose ethylene oxide chains are tightly associated with water molecules.

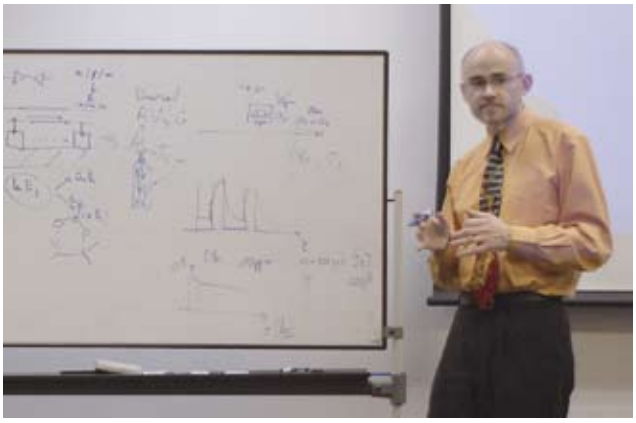

Figure 3. Professor Marcel Bouvet from ESPCI, France gave a stimulating seminar.

Properties and Specific Aggregate Structures, Grant-in-Aid for Scientific Research (2) on Priority Areas of Molecular Conductors, 17 October 2003–31 March 2008.

Asami K, Dielectric Monitoring of Cultured Cells Responding to External Stimuli, Collaboration Research with Sony Corporation (Life Science Laboratory, Material Laboratories), 28 June 2007–31 March 2008.