

Abstract: Infrared Spectroscopy of Self Assembled monolayers

Maciej Inerowicz

Self assembled monolayers are molecular assemblies formed by a process of spontaneous self-assembly of surfactant molecules on certain substrates. They can be prepared by using both a solution technique shown below (Figure 1) or by a vapor technique.

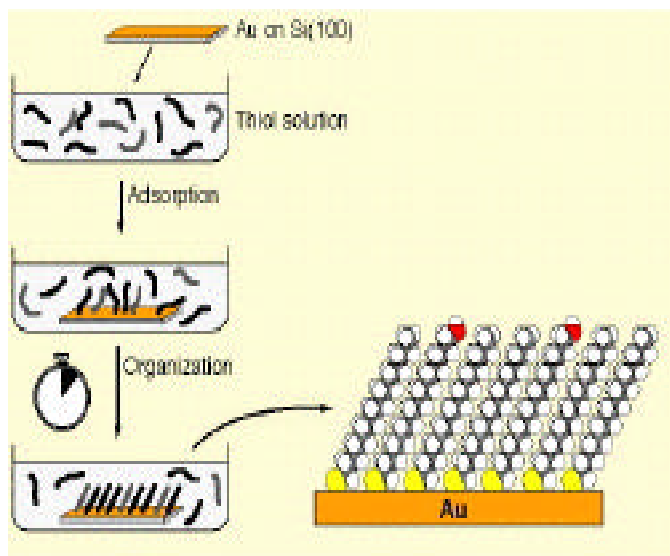


Figure 1

Research in the area of SAMS began in 1983 when Ralph Nuzzo and David Allara of Bell Laboratories first reported spontaneous adsorption of organic disulfides. Since then tremendous advancement have been made in the field which are reflected in the increased molecular complexity and control over monolayer structure. Advancements in the field and possible applications of these systems created enormous interest in SAMs which can be noted in the figure below (Figure 2)

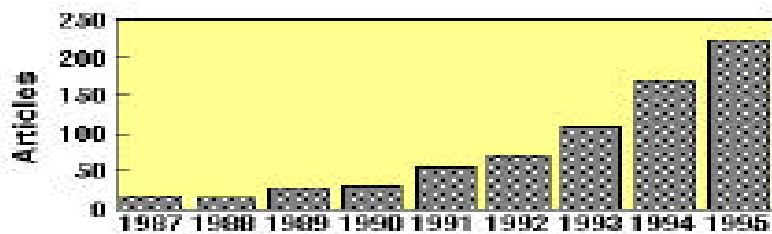


Figure 2. Number of published articles dealing with self-assembled monolayers per year, according to searches in the Chemical Abstracts and Science Citation Index databases.

The objective of my study was to gain valuable insight into the process of creating these structures as well as to produce valuable IR spectra of SAMs.

Molecules energy is quantized and it can only transition between these levels by absorbing or emitting energy in the form of electromagnetic radiation of particular frequency.

$$\nu = E/h \text{ cycles/sec}$$

Exposing the sample to IR light and detecting the relative intensities of particular frequencies of the IR light after it passes through the sample in comparison to initial intensities of these frequencies allows for the creation of an absorption spectrum.

Absorption peaks will appear at frequencies at which the molecule can absorb radiation and transition to a higher energy state. In order for the vibrating molecule to interact with radiation the molecule must have a change in the dipole moment.

The molecule Studied this summer was XYL(1,4-Benzenedimethanethiol) which readily adsorbs onto the gold-coated surface. The technique used to grow SAMs in our lab was the solution technique, which involves immersing a substrate into a solvent with the desired molecule.

XYL's vibrational modes can be related to the 30 normal vibrational modes of benzene. Most of these 30 vibrations are observed on solution XYL while only some appear on the SAM spectrum due to the presence of surface dipole selection rule. The IR technique used in our lab to do Vibrational Spectroscopy (IR) was RAIRS (reflection absorption infrared spectroscopy) usually used to study adsorbates on metallic surfaces.

This study used Wontaek's predictions on the location and type of molecular vibrations of XYL. The experimental absorption peaks were further analyzed and compared to the theoretical work done by Wontaek which also allowed determining the orientation of the molecular assemblies. Various experimental spectra obtained in lab had confirmed the presence of the desired molecule. The unexpected peaks may have been caused by contamination of the surface.