# Final Report for DOE PAIR Grant: Liquid film/polymer interfaces

**Grant Period**: 9/15/98-3/14/2003
**Grant Number**: DE-FG02-98ER45734
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**Originally to be in collaboration with**:

- York International Airside Products Division
  Contact: Charles H. Bemisderfer, product engineer
- DuPont Central Research and Development
  Contact: Dr. John Van Alsten (left DuPont in 2000)

**Objectives of Grant**:

1. Through experimental studies, advance the fundamental understanding of the principles that govern adsorption and wetting phenomena at polymer and organic surfaces.
2. Establish a firm scientific basis for improving the design of coatings for metal fin cooling surfaces used to control the wetting of water condensate for optimum energy efficiency.

**Project Personnel**:

| Name | Category | Current Status |
|---|---|---|
| Andy Hooper | Postdoc | Employed in industry |
| Tad Daniel | Grad Student | In chemistry PhD program |
| Matt Dixon | Grad Student | In chemistry PhD program |
| Matt Garrett | Grad Student | Graduated with MS degree |

## Summary


#### Industrial interactions

*DuPont*: This interaction was discontinued by Dupont. The original project contact, Dr. John Van Alsten at DuPont CR&D, left the company and the Company decided not to pursue the collaboration further. An interaction with Dr. Barry Lange at Rohm & Haas was formed. Rohm & Haas investigated coatings suitable for wetting control on aluminum cooling fins for York air conditioning products but discontinued the work on the basis that the market was not large enough to be profitable.

*York*: Interactions with Charles Bemisderfer and several of the engineers at York were discontinued temporarily in 2000 due to major reorganizations in the cooling fin area. Based on the progress of the earlier Penn State-York work, York planned on moving ahead with introducing a new, more energy-efficient air conditioning product in the near future. These plans were postponed until the engineering area was reorganized. The reorganization was done but the cooling fin project was dropped entirely and York discontinued the interaction with Penn State. During the active time of the intereaction cleaning methods were developed jointly by Penn State and York which looked promising to keep the cooling fins wettable without the need to use polymer coatings. This may have been put into production but the engineer who was originally assigned to the project moved on to other areas and no information is available. If implemented, in principle the development would lead to energy efficient fins that could be produced at a cost saving compared to polymer-coated fins.

#### Scientific Research

- Summary
  - *Ice Clustering*:
    Earlier work done with Professor Bo Liedberg (Linkoping U, Sweden) on the infrared vibrational analysis of the clustering of ice on self-assembled monolayers (SAMs) was to be analyzed using spectral simulation methods developed at Penn State. It was planned to have Liedberg and/or a graduate student come to Penn State for a month or two to work out the calculations. The student came and the calculations were completed. Upon returning to Sweden new systems were examined and further calculations done. Professor Liedberg decided to add more experiments and as of early 2003 was writing several manuscripts.
  - *Ambient Temperature $H_2O$ adsorption on SAMs*.
    **A.** A large amount of earlier infrared data had been taken of adsorbed water on a variety of SAMs, both hydrophilic and hydrophobic. The interpretation of the hydrophobic cases lead to the hypothesis of large (micrometer clusters) of ~monolayer coverages at saturation vapor pressure. This interpretation was quite controversial and sufficiently important that it led us to hold off publication of the data until an independent method could be found to characterize the water morphology. We investigated using synchrotron X-ray scattering at Argonne or Brookhaven but decided that these experiments were too difficult. Rather, we concluded that the most promising method for us is the use of non-contact capacitance AFM. Working with Miquel Salmeron at the DOE LBL lab, we constructed our own high precision

AFM and it now works extremely well for applications such as molecular resolution imaging of SAMs. We further constructed a UHV system with an STM and are now in the process of adding an AFM. Because of other priorities we were not able to get the water adsorption experiments running but the capability has been built.

**B.** Two small volume vacuum-vapor chambers interfaced with high precision and accuracy quartz crystal microgravimetry (QCM) devices were constructed for the measurement of variable temperature vapor adsorption on organic surfaces. A large amount of isotherm data was measured for a wide variety of chemically functionalized self-assembled monolayers and also oxide films. Mostly water vapor data were collected but also hexane and hexadecane were done.

**C.** A small volume vacuum-humidity chamber was built and designed to interface with a home built spectroscopic ellipsometer. Initial measurements were made of water isotherms on $SiO_2$ and the system gave results within experimental error of the QCM data.

**D.** A very small volume vacuum-humidity chamber was built and designed to interface with a FTIR spectrometer system built for high performance reflection experiments. Numerous problems with instrumental artifacts arose in this configuration and it was concluded that a larger volume chamber is required to be able to reproduce the original results, which were obtained in a large volume chamber. Since this chamber was reconfigured for metal vapor deposition experiments a new chamber needed to be built.

- Publications:
  - *Nucleation and Growth of Calcium Phosphate onto Self-Assembled Templates by a Solution-Formed Critical Nucleus Mechanism: Physiological Solutions*, B.J. Tarasevich, C.C. Chusuei, D.L. Allara, *J.Phys.Chem.B*., **in press**
  - *Calcium Phosphate Films by the Two and Three Dimensional Assembly of Nanoparticles onto Self-Assembled Monolayers*, B.J. Tarasevich, C.C. Chusuei, T.D. Daniel, D.L. Allara, ***J.Phys.Chem.B***,. submitted

  - E. Koo, M. Garrett and D. Allara, *The Structure of Chemisorbed Poly(acrylic Acid) Molecules on Aluminum Oxide*, in preparation
  - E. Koo, M. Garrett and D. Allara, *Wetting Properties of Chemically Modified Poly(acrylic acid) Thin Films on Aluminum Oxide*, in preparation
  - E. Koo, M. Garrett and D. Allara, *Correlations between Chain Conformation and Wetting Properties of Grafted Alkyl Chain Thin Film Structures*, in preparation
  - B. Liedberg, M. Garrett and D. Allara, *Clustering Phenomena of Low-Temperature Water Phases at Self-Assembled Monolayer Surfaces*, in preparation
  - T. Boland, M. Garrett, M. Dixon, A. Hooper and D. Allara, *Fundamental Studies of Equilibrium Water structures near Organic Surfaces. I. Rigid and close packed self-assembled monolayers*, to be submitted to *J.Phys. Chem. B.*
  - M. Garrett, M. Dixon, M. Saltzgueber, C. Rickard, K. Seshadri, M. Lercel, H.G. Craighead and D.L. Allara, *Restructuring Effects of Interfacial pH on n-Alkylsiloxane Monolayers on Solid Surfaces*
  - M. Garrett, K. Seshadri, A. Parikh, T. Courtney, M. Dixon, M. Lercel, H. Craighead and D. Allara, *Substrate-Independence via Interfacial Water in The Self-Assembly of n-Alkylsiloxane Monolayers on High Energy Surfaces*