

A Physiochemical Description of Three Interfaces; Nucleation Volume, Polymer-Metal Adhesion and Stern Adsorption Layer

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Abstract

Three critical interfaces in ink jet devices are briefly described and speculations about likely problems and the means of assessing these problems offered. The three interfaces include the nucleation volume; a polymer to metal interface and the interface derived from Stern layer adsorption. The impact of facilitated diffusion processes on the physiochemical properties of the interface is also discussed. Investigations of the interfaces by molecular level computational simulations are proposed.

Introduction

In this paper, three critical interfaces within an ink jet device will be described from a physiochemical perspective. The intent is to aid materials design engineers and scientist in their labor.

The nucleation volume is the effective interface where the initial energy transfer from the heater to the immediate fluid occurs. More efficient nucleation processes through better coupling of the heater surface to that of the contact fluid are proposed. Surface defects spaced 10-100-nm apart should measure at least 1-nm but less than 10-nm if improved nucleation processes are desired.

The second interface of interest is the physical volume near the polymer-oxide-ink or air adhesion joint. Two facilitated diffusion models for adhesion failure are presented to the designer. The first of these proposes a dissolution of the polymer-to-oxide bond that is facilitated by a diffusion process. The rates of diffusion are dramatically impacted by a chemical reaction. Upon the establishment of a chemical potential differentiation, 10^3 to 10^5 rate enhancements can be expected. Under these conditions the role of osmotic pressure should be considered as a driver for adhesion failure.

The final interface considered is that of a derived interface established after prolonged contact between two dissimilar dielectric materials. The designer is reminded of the Stern layer adsorption process in altering the wetting and subsequent performance of critical interfaces.

The Nucleation Process

For optimal device performance, a uniform vapor generation across the planar surface is desired. To achieve this uniformity, it is necessary to induce massive

heterogeneous nucleation over the entire surface. Current devices nucleate heterogeneously from only a few sites over the heater surface when water is utilized. Alcoholic solutions on the other hand form numerous sites of nucleation with no obvious correlation to particular sites on the surface. Various heater surfaces yield similar results for the two liquids suggesting that the relevant surface feature is not the chemical character of the site. The observations support the notion that the critical surface features involve shape or charge. Further, an observation that introducing particles (0.1 μm and larger) or roughing the surface does not affect the nucleating behavior, suggests that the spatial region of the site is small.

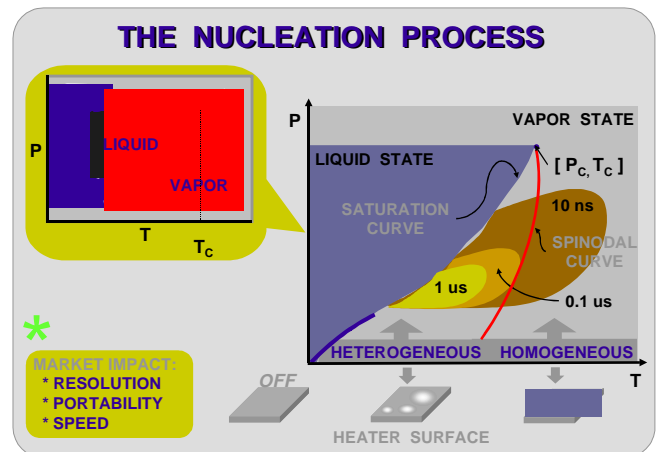


Figure 1. *p-T* diagram of the Nucleation Process

Figure 1 illustrates the nucleation process as a *p-T* diagram. For fast dT/dt conditions, homogeneous nucleation is depicted to the right of the spinodal line and molecular fluctuations are sufficient to cause nucleation of the fluid volume. For intermediate dT/dt conditions, density fluctuations in the liquid can spontaneously lead to bubble formation. This favors homogeneous nucleation in the bulk of the hot fluid volume. Such a process is perhaps operative for alcoholic liquids. The slow dT/dt conditions illustrated for rates of about 1- μs are common in commercially available ink jet devices.

Figure 2 depicts both the surface defect types that impact nucleation and the critical properties of water that

impact the spatial dimensions of the nucleation site. Investigations of the nucleation process are difficult or impossible analytically but modern computational tools can aid the designer greatly in this general field of interest.

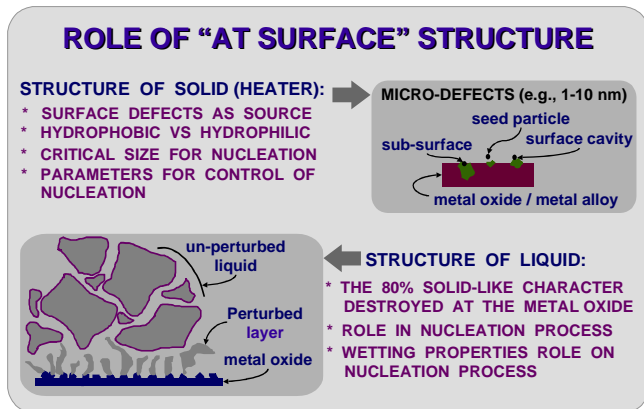


Figure 2. Microscopic structural considerations at the surface

Polymer to Metal Adhesion

The adhesion of a polymer to a gold or metal oxide surface is common to all ink jet devices. The polymeric thick-film laminate typically includes monomers, photoinitiators and other additives. This interface must be stable for years of exposure to aqueous based inks which also contain a number of organic solvents. An understanding of the interface, the adhesive / cohesive properties, and chemical potential within the perturbed layer near the metal or oxide surface is highly desired.

Figure 3 depicts schematically the gradient effect of establishing a chemical potential between the polymer bulk and the surface. This potential may serve to drive the formation of concentration gradients such as that depicted in Figure 4. Such gradients upon aging of the polymer result in polymer-polymer failures of the adhesion.

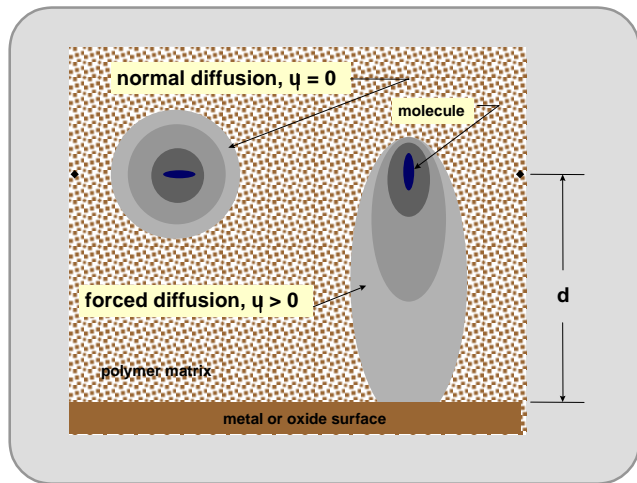


Figure 3. Facilitated diffusion process

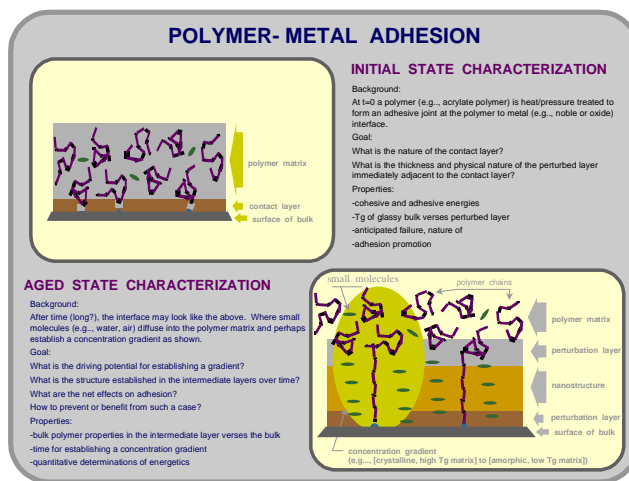


Figure 4. Polymer-polymer failure mechanism

In Figure 5, interface failure is the result of a facilitated diffusion of a plasticizing solvent from the ink formulation. Such agents may generate favorable osmotic pressures within the solvent depleted zone of the interface leading to an eventual general failure of the adhesive. Such failure mechanisms are difficult to investigate analytically but do lend themselves to modern computer simulations tools.

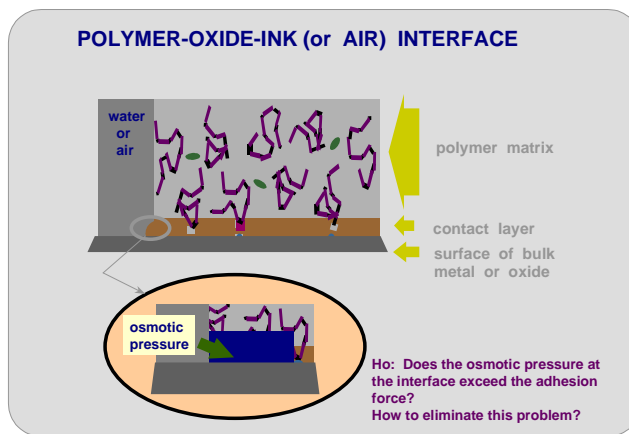


Figure 5. Dissolution of polymer-to-metal links

Stern Layer Adsorption

Once two dissimilar materials are placed in molecular contact with one another, a chemical potential is established. The magnitude and its impact on the diffusion of small molecules are important in building more reliable ink jet devices. Figure 6, illustrates schematically the formation of a Stern layer from the chemical potential differences of a liquid in contact with any solid. If conditions are right, such layers may lead to deposition and wetting property changes in the surfaces. The impact of the Stern layer adsorption on ink jet devices is presented and models for simulation presented.

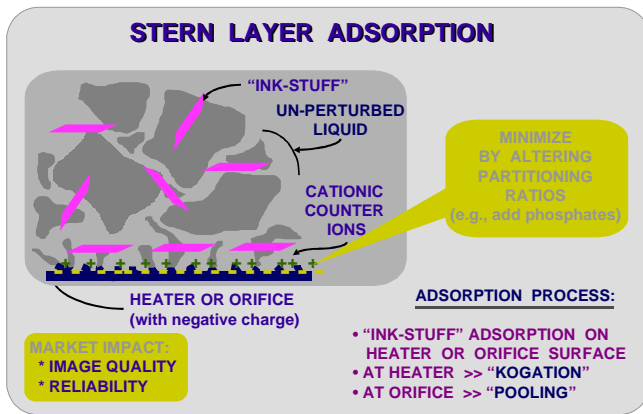


Figure 6. A Stern layer adsorption interface

Summary

The three interfaces described in brief form impact the operating efficiency, resolution and product life dramatically. In each case, the analytical evaluation of the interface performance is difficult or impossible. However, the advances in computational tools over the past 5-years make such problems manageable.

Biography

Dr. Miller has spent 12+ years with Hewlett-Packard Laboratories developing new printing technologies and theoretical underpinnings for various components of the Thermal Ink Jet (TIJ) technology group. Prior to joining HP-Labs, Dr. Miller led a team of technical contributors that led to the successful introduction of the first commercial TIJ printer. Since leaving HP-Labs, Dr. Miller founded RJM & Associates which consults in digital printing, computer simulations and micro-instrumentation.

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