Thermo-mechanical optimization of thermally actuated cantilever arrays

David Bullen*, Ming Zhang, Chang Liu
Micro Actuators, Sensors, and Systems Group, Micro and Nanotechnology Laboratory, Department of Electrical and Computer Engineering, University of Illinois at Urbana Champaign

ABSTRACT

Scanning probe lithography (SPL) is an emerging method of producing sub 50-nm features for semiconductor applications. A new variation of this process known as Dip Pen Nanolithography (DPN) expands the range of SPL capabilities to include depositing organic and biological macromolecules with nanometer precision. Recent work has been underway to implement DPN as parallel process by employing close packed arrays of individually thermally actuated DPN probes (TA-DPN arrays). In these types of devices, it is not necessary to have feedback control of the height of individual tips during operation. This simplifies the control system and probe structure but complicates array design because of the uncontrolled mechanical interaction between the tip and surface. We have found that TA-DPN arrays are subject to several failure modes that make optimization difficult, including surface scratching, excess tip angle, and problems resulting from inadequate actuation. In this paper, these performance issues are outlined and resolved with the creation of a multi-parameter simulator. The simulation predicts array behavior by employing engineering beam theory, Hertz contact mechanics, and capillary adhesion theory. Using the new insights gained from this simulation method, TA-DPN arrays can be quickly optimized based on any desired criteria.

Keywords: Dip Pen Nanolithography, scanning probe lithography, thermal actuator, AFM, simulation

1. INTRODUCTION

Scanning probe lithography is a core technology in the effort to reduce feature size in lithographic applications. Dip Pen Nanolithography\(^1\) (DPN) is a recent and innovative variation of this process. In this method, patterns are formed by the diffusion of a chemical species from an AFM probe tip to the substrate through the adsorbed water meniscus connecting the two. DPN is unique because it can be used to deposit organic and inorganic compounds as well as biological macromolecules on a variety of surfaces. It can be performed without the need for harsh conditions such as high vacuum or high electric fields, thus preserving the sensitive chemical species being deposited. DPN has been used to pattern thiol based self assembled monolayers for use as semiconductor processing resists\(^2\), and has achieved minimum line widths\(^3\) below 15nm.

As with all scanning probe lithographic methods, increases in speed can be achieved if the process is performed using many probes in parallel. In this respect, DPN has an advantage over other methods such as electric field oxidation of silicon. Some variations of the electric field method require the probes to be maintained a precise distance above the surface. This requires active feedback control of the height of each probe while scanning. With single probe devices, this is a straightforward task, but it becomes difficult when arrays of probes are implemented\(^4\). Since DPN operates with the probes in contact with the substrate, active height control is unnecessary. This allows large probe arrays to be used where each probe is supported by a soft cantilever that lightly presses the tip against the substrate. Passive arrays of such devices have already been realized\(^5,6\). To stop the lithographic process, thermal or electrostatic actuators can be added to the probes to lift individual tips off the surface. A feedback control system is not required for this task since the height of the actuated tip does not have to be maintained precisely.

As might be expected, these advantages come with a price. Since DPN arrays operate in contact mode, the mechanical interaction between the probe and surface is far stronger that in non-contact methods. Without control of individual tip height, adjacent probes in an array must accommodate misalignment and surface topology by passively deflecting against the substrate. Unless the array is appropriately designed, individual probes may scratch the surface or they may be unable to develop enough force to overcome surface adhesion. In many cases, these constraints conflict
with each other, making device optimization difficult. In short, the simplicity gained by eliminating individual tip control is paid for by the need to use arrays with carefully analyzed properties.

The purpose of this work is to identify and describe the major failure modes of DPN probe arrays and develop an analytical, multi-parameter simulation to quickly identify failure modes for design optimization. This work is primarily focused on devices consisting of arrays of thermally actuated DPN probes (TA-DPN arrays), although the principles are applicable to other types of contact-mode probe arrays. The task of the simulator is to rapidly evaluate large blocks of prospective array designs under a given set of fabrication and operating conditions. This information is then used to identify designs that are optimal for a specific set of those conditions.

2. ANALYSIS

In order to obtain a valid estimate of TA-DPN array performance, the analysis must include all of the vital aspects of the design problem. These include probe and array geometry, material properties, operating conditions, alignment tolerances, surface properties, and models of cantilever beams, adhesion, and surface scratching. The role and implementation of each of these aspects is described in this section.

2.1 Device layout

The layout assumed in this analysis is shown in Fig. 1. The design consists of an array of close packed rectangular cantilever probes that are configured as bimorph thermal actuators. TA-DPN arrays have several characteristics that make them promising for DPN applications including simple geometry, ease of fabrication, and a compact actuator that allows for high probe densities. The simulator calculates beam properties on a section-by-section basis from one end of the probe to the other. As a result, most thermal actuator layouts can be accommodated with minimal effort. In the layout used here, each probe has a thin film metal heater at its base, a metal actuator patch over much its remaining length, and a pyramid tip at the free end. The actuator patch is typically made of a high thermal expansion coefficient metal and is deposited at the same time as the heater and power leads. The films are stacked such that the tip moves away from the surface when heated.

The material system chosen is a vital simulation parameter. Each combination of high and low thermal expansion material has its own fabrication issues, operating range, and performance tradeoffs. These factors are
addressed in the analysis by limiting the geometry and operating conditions as necessary. For this work, the material system chosen was gold on silicon nitride. This system requires minimal effort to fabricate and produces effective, robust thermal actuators. The arrays are made by first etching silicon tips in a silicon wafer by anisotropic plasma or wet etching from the upper surface. Silicon nitride is then deposited on the substrate surface and the beams are patterned. The heater, leads, and actuator patch are produced by evaporating and patterning a chromium adhesion layer and gold layer using the same mask. The beams are finally released by anisotropic etching from the front side or backside of the wafer. This process results in probes having a thickness generally less than one micron and blunt tips with a radius of curvature equal to the beam thickness. Sharp tips are possible with a different, more complicated process. This process also results in a heater, leads, and actuation patch that have the same thickness. A more detailed description of this process can be found elsewhere.

The simulation works by iterating through and evaluating various beam geometries. The range of geometries must be decided before the analysis begins. This decision is strongly influenced by the material and fabrication process used. For this simulation, three variables were chosen with the following ranges: silicon nitride thickness 4000-10000Å, gold thickness 500-3000Å, and beam lengths of 100-500µm. These variables have the most significant impact on device performance. The beam lengths were limited to less than 500µm due to difficulties in drying longer beams after the final wet release step. The beam width was fixed at 80µm and the chromium thickness was fixed at 100Å.

2.2 Failure criteria

Contact mode lithographic arrays can produce unacceptable results for several reasons. We have found that TA-DPN arrays have five important failure criteria that can be evaluated in the design phase. Each criterion is a parameter that, when exceeded, could lead to unacceptable results during lithography. These criteria are: surface scratching, excess tip angle, overdrive, adhesion, and topography. Although not listed, excess temperature is also a failure mode. Excessive temperatures can alter DPN chemistry and cause changes in the microstructure of the actuator’s metal films. This criterion is automatically satisfied in the simulation by selecting an acceptable operating temperature before the simulation begins.

2.2.1 Overdrive criterion

Atomic force microscope (AFM) alignment plays an important role in TA-DPN array performance. When an array is installed in an AFM, there will always be a small amount of unavoidable angular misalignment between the plane swept out by the piezo, the sample surface, and the array. Without a control system to correct for this misalignment, the array must be pressed downward an additional amount beyond the point where the first tip makes contact to ensure all the tips touch the surface. This additional amount is defined as the array overdrive and is calculated from estimates of the minimum achievable array-to-surface misalignment, the array width, and the piezo scan size. Irregularities such as small variations in tip height must also be accommodated by the overdrive. This value is estimated by inspecting previously made devices.

Overdrive failures occur when the actuator cannot produce enough tip deflection to overcome the array overdrive. This prevents the tips from leaving the surface when actuated, making it impossible to suspend the deposition process. To evaluate this criterion, the thermal deflection of the beam is calculated using engineering beam theory, then compared with the array overdrive.

2.2.2 Topography criterion

The topography failure criterion is also evaluated from beam deflection. Topography violations occur when the probe can lift above the surface (the deflection exceeds the overdrive) but not rise high enough to clear topological features. When this occurs, high features will be inadvertently coated with chemical as the probe passes over them. This criterion is evaluated by comparing the tip deflection with the sum of the overdrive and maximum surface height. The maximum surface height is estimated from knowledge of the intended surface.

2.2.3 Adhesion criterion
The adhesion failure criterion is also related to the magnitude of the thermal deflection but requires more information to evaluate. The DPN process uses a water meniscus between the tip and substrate as the diffusion pathway for the deposited chemical. The meniscus exerts an adhesive force on the tip that must be overcome to actuate the probe. If the probe cannot produce enough force, the tip remains adhered to the surface and the deposition cannot be suspended. The force generated by the probe is evaluated from the distance it can move above the surface and the beam stiffness.

To begin the evaluation, the adhesive force must be estimated using thermodynamics. The shape of the axially symmetric liquid meniscus is known as a pendular ring and is shown in Fig. 2. Due to the meniscus surface tension, the capillary pressure is lower than the pressure of the surrounding environment. The differential pressure across the meniscus is related to its mean curvature by the Laplace equation8

\[ \Delta p = \frac{\gamma}{R} \]  

where \( \Delta p \) is the differential pressure across the meniscus surface, \( \gamma \) is the surface tension of the liquid, and \( R \) is the mean radius. The mean radius, also called the Kelvin radius, is found from \( 1/R = 1/r_1 + 1/r_2 \). The shape of the meniscus shown in Fig. 2 is approximate due to the assumption of a constant value for \( r_1 \) at every point on the surface. In a true meniscus, the mean radius of curvature \( R \) is constant over the entire surface, thus \( r_1 \) should change as \( r_2 \) changes at different points. Since analytical capillary force solutions based on the true meniscus shape9 are prohibitively complicated, a "circle approximation" is employed as shown in Fig. 2. It has been shown10 that assuming a constant value for \( r_1 \) is reasonably accurate in the range of relative humidity encountered during DPN (30%-70%). After making this approximation, the meniscus shape is found from the contact geometry, humidity, and surface parameters using the Kelvin equation10

\[ \frac{kT}{\nu_0} \ln \frac{P}{P_{sat}} = \frac{1}{r_1 + 1/r_2} + \frac{1}{R_{tip} \sin \phi} + \frac{\cos(\theta_1 + \phi) + \cos \theta_2}{h + R_{tip} (1 - \cos \phi)}. \]  

(2)

Here, \( k \) is the boltzmann constant, \( T \) is the temperature, \( \nu_0 \) is the molecular volume, \( P/P_{sat} \) is the relative vapor pressure (relative humidity), \( \theta_1 \) and \( \theta_2 \) are the contact angles of the meniscus fluid on the tip and substrate respectively, \( \phi \) is the filling angle, and \( R_{tip} \) is the radius of the tip. The sign of the meniscus radii is based on curvature with radii measured from the fluid side being positive and radii measured from the vapor side being negative. Once the meniscus geometry is known, the contribution to adhesion from surface tension and capillary pressure can be found using10,11

\[ F_{SurfaceTension} = 2\pi R_{tip} \sin \phi \sin(\theta_1 + \phi) \]  

(3)

and

\[ F_{Capillary} = \pi r_1^2 \Delta p. \]  

(4)

Adhesion contributions due to van der Waals forces and other surface forces can also be estimated using existing theories such as DMT contact analysis11. Unfortunately, this involves many poorly understood factors such as the effect of surface binding hydrophobic molecules, screening by the interfacial liquid, and the fact that the meniscus cannot maintain equilibrium while the probe is traversing the surface12. The effort to understand nanoscale contact adhesion is still an active area of research. This analysis is only expected to give a general idea of the magnitude of the adhesive force.

2.2.4 Tip angle criterion

The tip angle criterion is particularly important in thermally actuated probe designs. Tip angle violations result from excessive curling of the cantilever after release. Thermal actuators frequently suffer from post release curl due to deposition stress in their films and subsequent annealing during processing and operation. This curl can cause the tip to be deflected far out of the plane of the substrate, making the array unusable. A large tip angle will result in difficulty getting the tip on the surface, difficulty in obtaining a laser reflection from individual probes, and may cause a reduction in the effective lateral stiffness of the beam. The tip angle is calculated using engineering beam theory and a knowledge of the stress in each layer. The criterion is violated if it exceeds a maximum predetermined value.

2.2.5 Scratching criterion
The final criterion is surface scratching. Surface scratching results in excess tip friction, blunting, and is undesirable in DPN since the goal is to deposit chemicals without mechanically altering the surface. The scratching criterion is violated when the down force on the probe tip is sufficient to cause scratching. This criterion is difficult to evaluate analytically because sliding friction and surface roughness play a roll but their effect is hard to quantify. For the purpose of this simulation, a simple model was chosen. The maximum allowable tip down force is defined as the value required to reach full plasticity under the tip assuming Hertz contact mechanics. This occurs when the maximum stress under the tip reaches approximately three times the yield strength of the surface. For a spherical tip, this occurs at a tip load given by

\[
W = \frac{81R^2T^{3}Y^{3}}{16E^{2}}
\]

where \(Y\) is the yield strength of the surface, \(E^*\) is the reduced elastic modulus of the tip-surface system as given by

\[
\frac{1}{E^*} = \left(\frac{1-\nu^2}{E}\right)_{\text{Surface}} + \left(\frac{1-\nu^2}{E}\right)_{\text{Tip}}
\]

and \(\nu\) is the poisson’s ratio. Once the maximum value is found, the beam spring constant and overdrive are used to calculate the force exerted on the surface.

3. RESULTS AND DISCUSSION

The goal of this work was not to perform a parametric study of all possible array designs, but to examine a small set relevant to DPN applications. Due to the number of variables, a complete parametric study would be exceedingly large and of little importance. This analysis was restricted to 61,000 geometries in the length and thickness range defined in section 2.1. Although this is just one of many possible input sets, it effectively illustrates how array parameters affect the failure modes in conflicting ways and how designs can be optimized under these conditions. Throughout the rest of this section, every point in Figs. 3-8 represents an examined design and all plots have been given identical axis and perspective to allow for direct comparison.

Figure 3 shows the successful designs from the simulation run. Overall, 3,549 (5.8%) combinations did not fail any of the criteria described above. This may seem like a small percentage but this is actually a preferred result. If a simulation yields a large percentage of successful designs, then room exists for some criteria to be further restricted. For example, this simulation assumes that the thermal actuator operates with a temperature rise of 100°C. If a large number...
of successes had resulted, the operating temperature could be reduced to further constrain the design until only a small number of geometries succeed. These devices would represent designs optimized to run at low temperature. Any available design parameter may be used, separately or in combination, to limit the design. This allows the optimization to be based on any desired set of array properties and is one of the most powerful features of this simulation method.

In this simulation, the arrays have been optimized to produce the greatest possible force given the limits discussed above. As can be immediately seen, the successful designs are bounded by geometry (which is generally a representation of the limits on the fabrication process) and the different failure modes. There is no simple rule that describes the best design. We also see that accepting and fabricating the geometries with the maximum adhesion force is risky because they reside at the boundary of the acceptable set. Any variation in processing, layer thickness, or model error may result in a failure. A design in the center of the set is a better choice.

Figure 4 shows the designs that fail the substrate scratching criterion. This criterion is strongly affected by array overdrive, beam stiffness, tip radius, and substrate material. The concentration of failures at shorter, thicker designs indicates that beam stiffness is the dominant factor. This simulation is based on a gold substrate. Gold surfaces are popular in DPN due to the ease of forming thiol based self assembled monolayers on them. Gold is also a soft material with low yield strength, making substrate scratching a major problem. If a harder substrate such as silicon dioxide is assumed, arrays with stiffer beams and sharper tips can be used without violating the criterion.

Figure 5 shows the designs that fail the tip angle criterion. This failure mode is affected by the deposition stress and thickness of the constituent layers. In general, thermal actuators with layer thickness ratios that approach the optimal ratio will also have the worst curling problems. Thus, designing the most effective thermal actuator may result in a criterion violation, as it does here.

Figures 6 and 7 show the designs that violate the overdrive and topography criteria. These criteria are related as they indicate actuator designs that cannot deflect enough to overcome the overdrive, or overdrive plus surface topology respectively. The overdrive failure modes are strongly affected by the deflection of the thermal actuator, accuracy of the array alignment, and the magnitude of the tip-to-tip differences in height. Since DPN surfaces are generally very flat, there are very few topography failures and the plot is an extension of the overdrive failure plot.

Figure 8 shows the designs that violate the adhesion criterion. This failure mode is affected by almost every parameter in the array design. It is mainly a function of the meniscus area under the tip and thus the humidity. Since the
tip radius is equal to the thickness of the silicon nitride beam, beams with thicker layers experience more adhesion. The effect of increased length is more difficult to understand. Longer beams generate more deflection but are softer than shorter beams. Thus, without this analysis, it is difficult to see if lengthening the probes will improve the design. In this case, it does, but the improvement is small. This case illustrates the many conflicting behaviors that must be evaluated to produce a working TA-DPN array.

Fig. 7: Designs that pass the overdrive criterion but fail the topography criterion. The shading indicates the deflection deficiency in percent of the surface topographic height (2 µm in this simulation). Topography violations are an extension of the overdrive violations.

Fig. 8: Designs that pass the overdrive criterion but fail the adhesion criterion. The shading indicates the actuator force deficiency in percent of the tip adhesive force. At small tip sizes (i.e. small silicon nitride layer thickness) the failures are an extension of the overdrive failures. At large tip sizes, the capillary adhesive force grows roughly as the square of the tip size, resulting in more violations.

Overall, these results illustrate the significance of the design problem and the value of simulation. Although not as accurate as finite element models, the analytical method easily bundles together many different aspects of this multifaceted problem. Even though the use of analytical expressions can result in a loss of accuracy, it is an acceptable tradeoff for the vast increase in speed gained over FEA methods. In fact, the rapid pace of this simulation allows large blocks of designs be quickly evaluated using desktop computing power.

4. CONCLUSION

The critical factors in the design of TA-DPN arrays have been discussed. These devices are used to deposit organic and biological macromolecules on surfaces with nanometer precision. Since they do not require tip height control during lithography, they have a simple layout but require extreme care in their design due to the uncontrolled mechanical interaction between the probe and surface. The requirements for producing acceptable designs have been described and include eliminating problems due to surface adhesion, excess tip angle, array overdrive, surface topology, and surface scratching. An analytical simulation to evaluate and optimize potential designs was also discussed. The simulation is based on engineering beam theory, Hertz contact mechanics, and adhesion theory. It provides essential insights into array performance that would otherwise remain hidden and allows large sets of potential designs to be quickly optimized based on any design parameter.

ACKNOWLEDGMENTS

The authors would like to acknowledge support from the NSF Nanoscale Science and Engineering Center and the US Department of Defense under contracts ARMY NW 0650300F245h and NAVY CL 2468 ANTIC. They would also like to thank Dr. Sung-wook Chung for his assistance and insights.
REFERENCES


* contact dbullen@uiuc.edu; phone: (217)265-0808; fax: (217)244-6375; http://mass.micro.uiuc.edu; Micro Actuators, Sensors, and Systems Group, Micro and Nanotechnology Laboratory, University of Illinois at Urbana Champaign, 208 North Wright Street, Room 319B, Urbana, IL, USA 61801