Optimal Shape Design of Three-Dimensional MEMS with Applications to Electrostatic Comb Drives.

W. Ye* and S. Mukherjee*

*Department of Theoretical and Applied Mechanics
Kimball Hall, Cornell University, Ithaca, NY 14853

ABSTRACT

A methodology for solving inverse problems in Microelectromechanical (MEM) systems is proposed in this paper. Design of variable shape electrostatic comb drives (shape motors), in order to obtain desired force profiles, is presented as an application of the general methodology. This analysis includes simulation, sensitivity analysis and optimization.

A comb drive is one of the most important microactuators in MEM systems. In a standard comb drive, the capacitance varies linearly with displacement, resulting in an electrostatic driving force which is independent of the position of the moving fingers (relative to the fixed ones) except at the ends of the range of travel. It is of interest in some applications to have force profiles such as linear, quadratic or cubic. Such shaped comb drives could be useful, for example, for electrostatic tuning or to get actuators with longer ranges of travel than those of standard comb drives.

The present paper addresses the issues of simulation, sensitivity analysis, and then design (inverse problem) of comb drives with variable height profiles. Three-dimensional simulations of the exterior electrostatic field, and the resultant forces on the comb drive, are carried out with the exterior, indirect, boundary element method. Following direct simulation, sensitivity analysis is carried out by the direct differentiation approach. The variable of interest is the driving force while the design variables are parameters that determine the shape of the moving fingers. Next, an inverse problem is posed as follows: determine the height profile of the moving fingers such that the driving force is a desired function of the displacement of the comb drive. Comb drives of appropriate shapes, that produce desired force profiles, are obtained by this approach. Numerical results are given for shape motors that produce linear or cubic force profiles as functions of travel. The optimization code "E04UCF", from the NAG package, is used for this phase of the work.

Keywords: shaped comb drive, sensitivity, optimization, boundary element method

INTRODUCTION

It is perhaps fair to say that, to date, much of research and development effort in Micro-electro-mechanical (MEM) systems has been directed at fabrication and testing of these miniature devices. Nevertheless, analysis and computer simulation of MEM structures is also an active field of research (see, for example, [1]). There are at least two commercially available MEMS simulation tools. One is MEMCAD from Microcosm Technology Inc. It is an integrated package for mask layout, fabrication process description, geometric modeling, electro-mechanical simulation, and results visualization. Some work based on MEMCAD has already been reported recently [2]. Another commercially available package is IntelliCAD from IntelliSense Corp. which includes both commercial and custom tools and databases. These commercially available CAD systems applicable to MEMS are primarily aimed at simulating fabrication processes and electro-mechanical behavior of a given design. Parametric optimization of a design for specified requirements is not feasible except by iterating the simulation over many input data sets - which is computationally expensive and time consuming. The optimal design methodology presented in this paper is quite general and can be applied to a wide variety of MEM structures. Shape design of a specific very important MEM device, a comb drive is presented here as the primary application of this design methodology. Design of a two-dimensional comb drive has been presented before [3]. A fully three-dimensional shape optimization problem is solved in this paper.

Comb-drive actuator is one of the most important actuators in MEM systems. In a typical comb drive, the capacitance is linear with travel δ, resulting in an electrostatic driving force which is independent of the position of the moving fingers (relative to the fixed ones) except at the ends of the range of travel. It is of interest in some applications to have force profiles such as linear, quadratic or cubic. One example is that, in many actuator applications, large displacement motion is highly desirable. However, the actuator springs exhibit nonlinear response for large displacements. The spring restoring force behaves as $R = k_1 x + k_2 x^3 + \cdots$, where x is the displacement and k_i are the spring constants. A large driving force is required in order to overcome the nonlinear restoring forces. Hence, a prohibitively large voltage must be applied on conventional comb actuators in order to achieve a large range of motion. It is therefore desirable to have variable shape comb drives such that the corresponding driving force profiles have similar nonlinear terms in x as does the restoring force, for a given applied voltage.

Another example of use of a variable shape comb drive is related to tuning MEMS. A comb drive with linear, quadratic or cubic force profile can be used for electrostatic tuning. In many MEMS applications, micromechanical resonators play an important role. In such devices, independent tuning of linear or nonlinear stiffness coefficients is an important issue [4].

Recently, a fringe field comb drive and a linearly varied length comb drive have been fabricated for electrostatic tuning by Adams *et al.* [4] and Lee *et al.* [5] respectively. In the device of Adams, the operation range of this device is limited to only within $2 \sim 5\mu m$, while, in Lee's device, only the linear stiffness can be tuned. So a large range comb drive which can be used to tune linear, quadratic and cubic stiffness, is highly desirable.

Comb drives with linear, quadratic and cubic force profiles have already been designed [3]. These designs, based on two-dimensional analysis, have uniform height profiles but variable gap profiles. Fabrication of such devices are underway at the Cornell Nanofabrication Facility. One disadvantage in such devices is area loss. In order to overcome this disadvantage, a different approach is presented in this work. Instead of changing gap profiles, the height profile of the moving fingers is changed. This results in a three-dimensional analysis and designs based on this approach do not have any area loss. Even though the final design can not be fabricated at present due to limitations of current manufacturing techniques, it nevertheless provides a very attractive alternative design.

The present paper addresses the issues of simulation, and then design (inverse problem) of comb drives with variable height profiles. Three-dimensional simulations of the exterior electrostatic field, and the resultant forces on the comb drive, are carried out with the exterior, indirect, boundary element method. Following direct simulation, sensitivity analysis is carried out by the direct differentiation approach (DDA [6]). The variable of interest is the driving force while the design variables are parameters that determine the shapes of the moving fingers. Next, an inverse problem is posed as follows: determine the height profile of the moving fingers such that the driving force is a desired function of the travel of the comb drive. Linear, quadratic and cubic functions are considered in this work. The optimization code "E04UCF" from the NAG package (http://www.nag.co.uk) is used for this phase of the work.

PROBLEM FORMULATION

A comb drive can be modeled as several conductors embedded in a uniform lossless three dimensional dielectrical medium. The electrostatic potential ϕ in the region exterior to the conductors satisfies the Laplace equation [7].

$$\nabla^2 \phi = 0 \tag{1}$$

On each conductor, the potential ϕ is a constant.

$$\phi = \phi_i, \qquad i = 1, 2, \cdots, m \tag{2}$$

where m is the total number of conductors.

For three-dimensional problems, the potential goes to zero at the infinity.

$$\phi_\infty = 0 \tag{3}$$

The electric charge distributes itself only on the surface of each conductor. The charge density is defined as

$$q_i(\mathbf{r}) = \epsilon \frac{\partial \phi_i(\mathbf{r})}{\partial n} \tag{4}$$

where $q_i(\mathbf{r})$ is the surface charge density at point $\mathbf{r}$ on the surface of conductor i, ϵ is the dielectric constant of the medium, ϕ_i is the electrostatic potential of conductor i and $\mathbf{n}$ is the inward normal to that conductor at point $\mathbf{r}$.

The surface force acting at a point on a conductor surface is given by the equation (refence [7])

$$\mathbf{f} = -\frac{1}{2}\frac{q^2}{\epsilon}\mathbf{n} \tag{5}$$

Therefore, the total force acting on the moving part of a comb drive is the integral of the surface forces over the entire surface of the moving part of the devices

$$\mathbf{F} = \int_\Gamma \mathbf{f} ds \tag{6}$$

while the driving force acting on the moving fingers along the x-direction (travel direction) is

$$F_x = \int_\Gamma f_x ds \tag{7}$$

Here f_x is the x-component of surface force $\mathbf{f}$ and Γ is the total surface of all the moving fingers. This driving force F_x depends on both the shape parameters of the fingers, as well as on the position δ of the moving fingers.

The design of a variable shape comb drive, with linear, quadratic or cubic (or some other prescribed function) driving force, can be posed as an optimal design problem. The goal of the optimization procedure is to minimize an objective function without violating the specified constraints.

The optimization problem is set up as

$$\begin{cases} \text{minimize} & \psi(c_i) \\ \text{subject to} & a_j(c_i) \leq 0 \end{cases} \tag{8}$$

where the objective function ψ is chosen as the integral of the square of the difference between the actual and desired force profiles, over the range of operation of the comb drive, i.e.

$$\psi(c_i) = \int_{\ell_1}^{\ell_2} (F_x(c_i,\delta) - F_e(\delta))^2 \, d\delta \tag{9}$$

Here, c_i are the parameters that define the shapes of the fingers of the comb drive, F_x is the driving force, δ is the position of a moving finger, $F_e(\delta)$ is the desired force profile that can be linear, quadratic or cubic (such as the driving force needed to counteract the cubic restoring force of nonlinear actuator springs.), ℓ_1, ℓ_2 are the initial and final positions of a moving finger and a_j are the constraints imposed by practical design issues.

SENSITIVITY ANALYSIS AND OPTIMIZATION PROCEDURE

An indirect boundary element method is used to solve equation (1) together with boundary conditions (2) and (3). The boundary integral equations for solving the charge density q are

$$\phi_i = \sum_{j=1}^{m} \int_{\partial s_j} \frac{q(\mathbf{r}')}{\epsilon}(\mathbf{r}')G(\mathbf{r},\mathbf{r}')ds(\mathbf{r}'), \quad i = 1,2,\cdots,N \tag{10}$$

where $\mathbf{r}$ is the position vector of source point located on conductor i, $\mathbf{r}'$ is the position vector of field point, G is the Green's function which is equal to $\frac{1}{4\pi\|\mathbf{r}-\mathbf{r}'\|}$ in 3-D, ∂s_j is the surface of conductor j and N is the total number of nodes.

A discretized version of equation (10), following standard procedures, is

$$\mathbf{A}\mathbf{q} = \boldsymbol{\phi} \tag{11}$$

where $\boldsymbol{\phi}$ is prescribed and $\mathbf{q}$ is the unknown vector.

The "analytical" gradient (sensitivities) of the function ψ with respect to the shape parameters c_i is used to solve the optimization problem. This gradient is obtained by the direct differentiation approach (DDA). There are several advantages of using the DDA for this problem, the most important being the higher accuracy this method delivers compared to the finite difference method. By taking the direct derivative of equations (10) with respect to the shape parameters and solving the resultant equations, the design sensitivity coefficients (DSCs) have the same accuracy as the physical quantities (ψ), while the accuracy of DSCs obtained by the finite difference method is one order lower than that of the physical quantities. Another advantage is related to computing efficiency. After discretizing the resultant integral equations, the linear system obtained has the same coefficient matrix A (see Equation (11)) as the one obtained for the calculation of the physical quantities. Only the right hand side vector needs to be recalculated.

The equations for obtaining the sensitivity of the charge density q with respect to a design parameters c, obtained by differentiating equation (10) with respect to c, are

$$\begin{aligned} \sum_{j=1}^{n} \int_{\partial s_j} \overset{*}{q}(\mathbf{r}')G(\mathbf{r},\mathbf{r}')ds(\mathbf{r}') = \\ -\sum_{j=1}^{n} \int_{\partial s_j} q(\mathbf{r}') \overset{*}{G}(\mathbf{r},\mathbf{r}')ds(\mathbf{r}') \\ -\sum_{j=1}^{n} \int_{\partial s_j} q(\mathbf{r}')G(\mathbf{r},\mathbf{r}')\overset{*}{ds}(\mathbf{r}') \end{aligned} \tag{12}$$

where $* \equiv \frac{\partial}{\partial c}$, with c being one of the c_i's. In the above, $\overset{*}{q}$ is the unknown function, $\overset{*}{G}$ can be easily obtained from G and $\overset{*}{ds}$ is available in many references.

A discretized form of (12) is

$$\mathbf{A}\overset{*}{\mathbf{q}} = \mathbf{b} \tag{13}$$

From equation (5), the sensitivity of the x-component of surface force f_x with respect of c can be obtained as

$$\overset{*}{f}_x = -\frac{q\,\overset{*}{q}}{\epsilon}n_x - \frac{1}{2}\frac{q^2}{\epsilon}\overset{*}{n}_x \tag{14}$$

Also, the sensitivity of driving force F_x can be calculated by differentiating equation (7) with respect to c

$$\overset{*}{F}_x = \int_\Gamma \overset{*}{f}_x \, ds + \int_\Gamma f_x d\overset{*}{s} \tag{15}$$

Finally, the sensitivity of the objective function ψ with respect to a design variable c is

$$\overset{*}{\psi} = \int_{\ell_1}^{\ell_2} 2\,(F_x(c_i,\delta) - F_e(\delta))\, \overset{*}{F}_x \, d\delta \tag{16}$$

Clearly, $\overset{*}{f}_x$, $\overset{*}{F}_x$ and finally $\overset{*}{\psi}$, for a specified configuration of the comb drive, can be obtained once the charge distribution q, its sensitivity $\overset{*}{q}$, as well as the geometry and the geometric sensitivities $\overset{*}{n}_x$ and $d\overset{*}{s}$ are known.

The optimization problem is solved by using the optimization code "E04UCF" from the NAG Fortran Library. This code is designed for solving nonlinear programming problems — minimization of a smooth nonlinear function subject to a set of constraints on the variables, either linear or nonlinear. In this particular problem, the constraints are linear.

E04UCF implements a sequential quadratic programming (SQP) method (Fletcher [8]). The basic structure of E04UCF involves *major* and *minor* iterations. The *major* iterations generate a sequence of iterates $\{\mathbf{c}_k\}$ that converge to $\mathbf{c}^*$, a first-order Kuhn-Tucker point.

At a typical major iteration, the new iterate $\bar{\mathbf{c}}$ is defined by

$$\bar{\mathbf{c}} = \mathbf{c} + \alpha \mathbf{p} \tag{17}$$

where $\mathbf{c}$ is the current iterate, the non-negative scalar α is the step length and $\mathbf{p}$ is the search direction. Also associated with each major iteration are estimates of the Langrange multipliers and a prediction of the active set (the set in which all the constraints are active, i.e. satisfied exactly).

The search direction $\mathbf{p}$ in (16) is the solution of a quadratic programming subproblem of the form

$$\begin{cases} \text{minimize} & \mathbf{g}^T\mathbf{p} + \frac{1}{2}\mathbf{p}^T\mathbf{H}\mathbf{p} \\ \text{subject to} & a_j(\mathbf{p}) \le -a_j(\mathbf{c}) \end{cases} \tag{18}$$

where $\mathbf{g}$ is the gradient of ϕ at $\mathbf{c}$ and the matrix $\mathbf{H}$ is a positive-definite quasi-Newton approximation to the Hessian of the Lagrangian function. The BFGS formula (Dennis *et al.* [9]) is used to update this matrix $\mathbf{H}$.

This quadratic programming subproblem is solved by a two-phase quadratic programming method. The two phases of the method are: finding an initial feasible point by minimizing the sum of infeasibilities (the feasibility phase), and minimizing the quadratic objective function within the feasible region (the optimality phase). In general, this must be done by iterations. These iterations are the *minor* iterations in E04UCF.

Once $\mathbf{p}$ has been computed, the major iteration proceeds by determining the Lagrangian merit function, which is the objective function ψ itself in the linear constraints case. Finally, the approximation to the transformed Hessian matrix is updated using a modified BFGS quasi-Newton update to incorporate new curvature information obtained in the move from $\mathbf{c}$ to $\bar{\mathbf{c}}$.

NUMERICAL IMPLEMENTATION AND RESULTS

Simulation of the driving force

The system of equations (11) resulting from the discretization of equation (10) is solved by LU decomposition. In order to save computing time, the matrix $\mathbf{A}$ is stored in LU form for future use in sensitivity calculations. All the weakly singular integrals appearing in the matrix $\mathbf{A}$ are evaluated by a mapping method proposed by Nagarajan *et al.* [10]. The regularized integrals are calculated using Gaussian Quadrature.

Numerical results for the driving force produced by a standard (uniform) comb drive, as a function of the distance traveled by the moving fingers, are shown in Figure (1), together with the results from two dimensional simulation of the same structure [3]. As expected, the driving force remains constant during most of the travel range because the gap between the fixed fingers and the moving finger is constant, and so are the heights of these fingers. When the moving finger is fully inserted into the fixed fingers, the electrostatic potential blows up due to contact between these two sets of fingers. The difference between these two results is around 5%. The results from the three dimensional model are slightly higher than the results from two dimensional model. This is because in 3-D model, in addition to the local fringe field, the global fringe field is also considered.

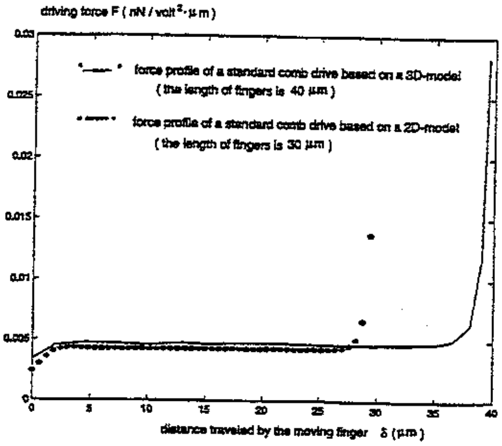

Figure 1: Driving force profiles of a standard comb drive based on the 3D and the 2D models.

The comb drive of interest in this work has uniform gap profile but a varying height profile. In order to have a polynomial driving force, the height profile of the moving finger is proposed to be a polynomial function, while the gap between the fixed and the moving fingers is a constant.

In this work, it is assumed that the shapes of the fixed fingers are fixed, while the shape of the moving finger can be varied. Figure (2) shows the three-dimensional shape of a proposed moving finger and its projection onto the $y = -1$ plane. This structure is symmetric about $z = 5$. The upper curve between a and b is a polynomial function of x

$$z_u = c_0 + c_1 x + c_2 x^2 + c_3 x^3 \tag{19}$$

where c_0, c_1, c_2, c_3, are design variables.

The lower curve is simply set as

$$z_l = 10 - z_u \tag{20}$$

to maintain the symmetry about the plane $z = 5$. The left and the right lines are $x_l = 1$ and $x_r = 40.5$, respectively. Between these lines, hermitian curves are used to smooth the corners. This is done for the purpose of avoiding the corner singularities exist in the exterior potential problems. The edges in the lateral plane are rounded off by semi-circles because of the same reason. It is important that edges and corners remain rounded after subjecting a structures to geometric perturbations.

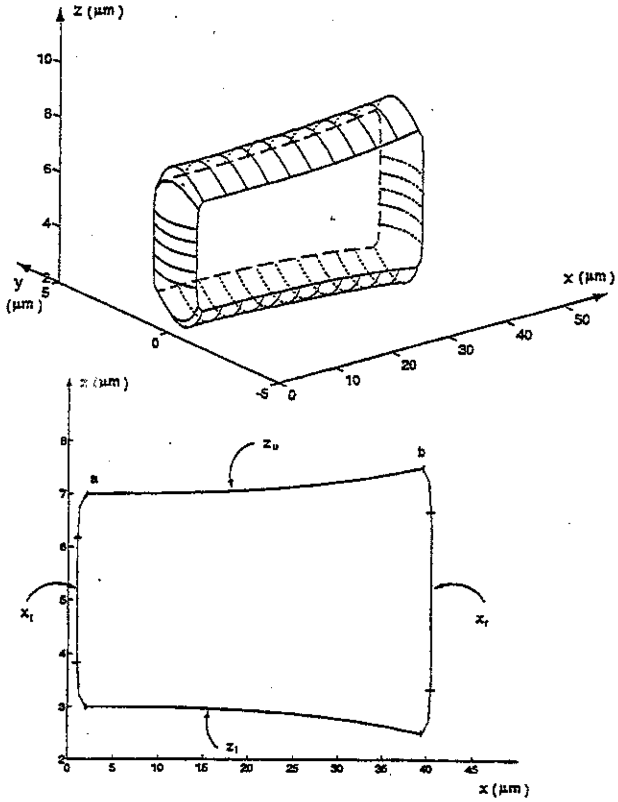

Figure 2: A 3D picture of the shape of a moving finger with variable height and its projection in $y = -1$ plane.

Sensitivity analysis

Equation (12) is solved by the usual boundary element method. As mentioned before, the matrix obtained from equation (12) is the same as the one obtained from equation (10) (please see equations (11) and (13)). Only the right-hand side in equation (13) needs to be recalculated. This right-hand side involves the sensitivities of nodal coordinates (in the $\overset{*}{G}$ function) that must be calculated carefully. A consistency must be maintained before and after perturbation of the geometry.

Table (1) shows the sensitivities of the objective function ψ with respect to the design variables c_i obtained from the direct differentiation and finite difference methods respectively for the case where $c_0 = 7.0, c_1 = 0.0, c_2 = 0.0, c_3 = 0.0$ and $\delta = 20\mu m$. After carefully choosing the perturbation step sizes in finite difference method, the differences between two sets of results coming from different methods are very small.

Table 1: The sensitivities of ψ with respect to $c_i, i = 0, 1, 2, 3$ obtained from DDA and FDM

	$\frac{\partial\psi}{\partial c_0}$	$\frac{\partial\psi}{\partial c_1}$	$\frac{\partial\psi}{\partial c_2}$	$\frac{\partial\psi}{\partial c_3}$
DDA	-1.24×10^{-3}	-0.0204	-0.349	-6.874
FDM	-1.24×10^{-3}	-0.0202	-0.3477	-6.867

Inverse problem

The goal here is to design a comb drive that has a polynomial force profile as a function of the distance traveled by its moving fingers. So the desired force profile $F_e(\delta)$ in equation (8) is set as a polynomial function of δ. For the purpose of illustration, only one example is shown in this section. In this example, a cubic force profile is chosen as the desired force profile

$$F_e(\delta) = 5.0 \times 10^{-7}\delta^3 + 3.8 \times 10^{-2} \tag{21}$$

The initial guesses for the design variables c_i are:

$$c_0 = 7.0, \quad c_1 = 0.0, \quad c_2 = 0.0, \quad c_3 = 0.0 \tag{22}$$

i.e. the initial shape of the comb drive is uniform.

Due to limitations of manufacturing techniques, the maximum height of the moving finger is set as $30\mu m$. This provides constraints on the design variables c_i, i.e.

$$c_0 + c_1 x + c_2 x^2 + c_3 x^3 \leq 30 \tag{23}$$

Also, at points a and b in Figure (2), the minimum values of z_u are set as $6.5\mu m$ and $7.5\mu m$ respectively, to ensure that the height of the moving finger is at least $5\mu m$.

Figure (3) shows the projections in the $x - z$ plane of the initial and final shape of the moving finger with cubic force profiles. The force profile of the comb drive at its initial shape, two intermediate shapes, and the final shape, are also shown there.

Each iteration needs 2 hours of CPU time on one node of an IBM SP2 computer. Also, convergence of the optimization problems would require a large number of iterations. Due to limitations of computing resources, these minima were not achieved - instead, the calculations were terminated when the magnitude of $Z^T\nabla\psi$ became sufficiently small. Here Z is a matrix whose columns form an orthogonal basis for the set of vectors orthogonal to the space spanned by the active constraints. Table (2) shows $\|Z^T\nabla\psi\|$ at the final designs. Of course, $\|Z^T\nabla\psi\|$ should be zero when ψ achieves its minimum. Also, the values of ψ at the final designs are shown in Table (2). From a practical point of view, the design shown in Figure (3) is adequate.

Following the exact same procedures, comb drives with linear, quadratic force profiles can be designed. These comb drives, plus the one shown above, together

Table 2: The values of the normal of the projected gradient and the objective function at the initial and the final designs

		$\|Z^T \nabla \psi\|$	ψ
Cubic	initial design	0.12	1.62×10^{-4}
Motor	final design	0.0001	2.4×10^{-6}

with the standard comb drive, serve as fundamental comb drives. These fundamental comb drives can be arranged in parallel , with suitable bias voltages applied to each comb drive, in order to obtain any desired polynomial (up to cubic) force profile.

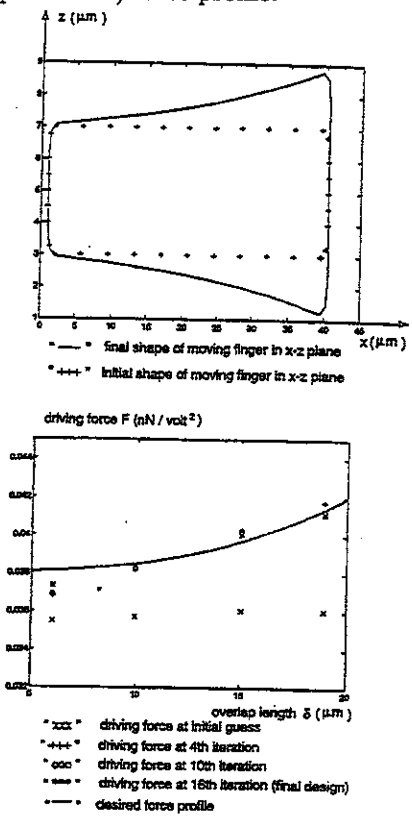

Figure 3: Cubic motor: Initial and final shapes of the moving finger in the x-z plane and the force profiles from this comb drive at different iterations.

CONCLUSIONS

A methodology for solving inverse problems in MEM systems, with the applications to variable shape electrostatic comb drives, is presented in this paper. This method is fairly general and can be applied to a wide variety of MEMS structures.

It is shown in this paper that, by solving an appropriate inverse problem, comb drives with variable height profiles can be designed that will deliver desired driving force profiles. Such comb drives occupy the same area as do standard comb drives. Thus, there is no any area loss in these designs.

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