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TOPOLOGY OPTIMIZATION OF MICROMACHINED STRUCTURES WITH SURFACE MICROMACHINING MANUFACTURING CONSTRAINTS

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ABSTRACT
Topology optimization methods have been shown to have extensive application in the design of microsystems. However, their utility in practical situations is restricted to predominantly planar configurations due to the limitations of most microfabrication techniques in realizing structures with arbitrary topologies in the direction perpendicular to the substrate. This study addresses the problem of synthesizing optimal topologies in the out-of-plane direction while obeying the constraints imposed by surface micromachining. A new formulation that achieves this by defining a design space that implicitly obeys the manufacturing constraints with a continuous design parameterization is presented in this paper. This is in contrast to including manufacturing cost in the objective function or constraints. The resulting solutions of the new formulation obtained with gradient-based optimization directly provide the photolithographic mask layouts. Two examples that illustrate the approach for the case of stiff structures are included.

INTRODUCTION
The microfabrication technology has spearheaded a revolution in the development of small and inexpensive devices that suit the growing demand for multi-functional, integrated systems through miniaturization. In contrast to many machining techniques at the macro scale, microfabrication has many limitations in terms of kinds of structures and features that can be economically realized. However, this has not stifled the ingenuity of engineers in coming up with innovative designs in microelectromechanical systems (MEMS) to achieve the desired functionality within the given manufacturing constraints. The advent of optimal topology optimization methods has further widened the scope for the microsystem designer in generating design concepts that are far from intuition [1, 2]. They also significantly reduce the tedium of trial-and-error based design.

Photolithography-based micromachining methods are amenable for realizing almost any geometric form in a plane and are limited only by their resolution. Therefore, they are very well suited for implementing optimal solutions that arise out of topology optimization performed on 2D domains. But not all microsystem components have vertically extruded shapes based on a planar geometry. Even a simple fixed-fixed beam made using surface micromachining [3] will have a 3-D shape due to its anchoring to the substrate with a gap underneath. Microfabrication methods do not allow arbitrary shapes in the out-of-plane direction perpendicular to the substrate. Furthermore, when a process is chosen, the thicknesses of layers in a multi-layer process are fixed, thus further constraining the designs. In order to perform topology optimization of structures in this direction, we must therefore suitably constrain the algorithm to search for solutions that conform to the manufacturing restructions. This is the focus of this paper.

At the macro scale too, human intervention is often required to modify the optimal topology to suit a manufacturing technique while retaining the key aspects of the design to the extent possible. However, this post-processing may lead to sub-optimal solutions. Thus, incorporating manufacturing constraints and cost into the topology optimization problem at the outset is equally relevant to macro-scale structures as it is for the microsystems. This is attracting increasing attention by researchers in academia [4-12] and industry [13, 14] who are working on macro-scale structures. The reported approaches include: making the post-processing systematic and efficient [4, 5], imposing a minimum length scale [6, 7], avoiding point flexures that are impractical [8], and two-stage methods or those that are specific to a manufacturing technique. The examples of the last category of methods include those specific to molding [9, 10], casting [11] and abrasive water-jet cutting [12]. Ad hoc and restrictive methods such as limiting the topologies to extruded designs, specific draw directions, etc., are also followed.

The above approaches have not yet been applied to topology optimization of micromachined structures. In the following sections, we describe a generic scheme for including surface micromachining constraints in topology optimization. Surface micromachining is substantially different from extrusion, molding, stamping, casting and other macro manufacturing methods. So, the method presented here is not an adaptation of any of the above methods. In fact, as will be explained later, we focus on defining a design space through a novel design parameterization that intrinsically obeys manufacturing constraints. Thus, we are not just posing a problem that minimizes the manufacturing cost or imposes manufacturing restrictions as constraints. This subtle difference makes this method applicable to many types of problems and makes it computationally efficient because multi-criteria objectives and multiple constraints are known to lead to algorithmic difficulties.

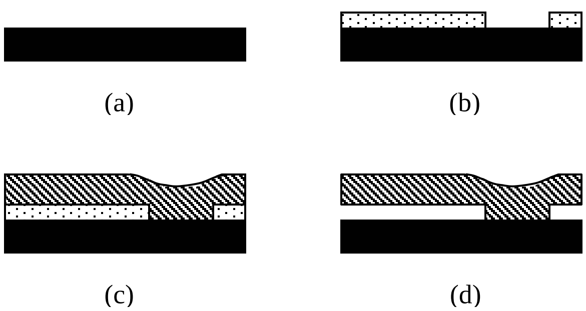

Figure 1. A simple surface micromachining process sequence. (a) Substrate wafer (b) Deposition of sacrificial oxide (c) Polysilicon structural layer (d) Oxide etch to release cantilever

In this paper, for the purpose of illustration, we consider the most familiar problem of topology optimization of obtaining the stiffest structure with a given volume of material and boundary conditions (loads and specified displacements). By keeping the manufacturing constraints in mind, we reformulate the problem using a new set of design variables. This alternative formulation is explained in the next section after a brief description of the surface micromachining and the optimization problem solved in this paper. Although we have chosen to deal only with structural optimization here, the same formulation may be applied to most multidisciplinary problems with additional effort in implementation.

Surface micromachining

There are a large number of micromachining processes used for the fabrication of MEMS devices. The most popular among them that are widely used in the industry and academia are surface and bulk micromachining. In this paper, we choose surface micromachining. This choice is attractive because surface micromachining is the most important micro-foundry process in the industry today (e.g., [15]).

In surface micromachining, alternate layers of polysilicon and sacrificial silicon oxide are used to define the device structure. While polysilicon serves as the structural material, silicon oxide is used as a sacrificial layer between the polysilicon layers and is etched away at the end of the procedure to create gaps and release the polysilicon layers. Following the deposition of each layer, photolithography is used to define relief features by masking/protecting certain regions while etching away the others. The combination of repeated deposition steps and photolithography produces useful structures like cantilevers, hinges, gears, etc. Figure 1 shows an example of this process where a sequence of four steps is used to make a simple cantilever. It is important to note that since both polysilicon and oxide layers are alternately deposited material layers of certain thickness, the relief features that are created by photolithography and etching in an individual layer are propagated through the successive layers. This leads to a complex topography. It was shown in [16] how a surface-micromachined component of valid topography can be used to synthesize its lithography mask layouts. The present approach to design parameterization builds upon that work.

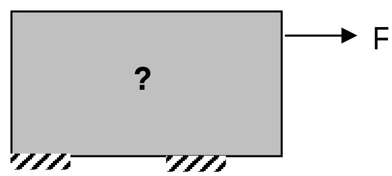

Figure 2. Specification for the topology optimization problem of stiffest structures

Topology optimization problem statement

The problem of generating the stiffest structure may be formally stated as one where we seek the optimal structure which has the least strain energy under the specified boundary conditions (BCs) using a given volume of material in a given domain (see Fig. 2). Mathematically this may be stated as follows.

$$\begin{aligned} \underset{\gamma}{Min}: \quad & SE(\gamma) = \frac{1}{2}\int_{\Omega} S(\gamma)\{\boldsymbol{\varepsilon} : \mathbf{E} : \boldsymbol{\varepsilon}\}\, d\Omega \\ s.t \quad & \nabla \cdot \left(S(\gamma)\mathbf{E} : \boldsymbol{\varepsilon}\right) = \mathbf{f} \quad \& \ BCs \\ & \int_{\Omega} \mathrm{V}(\gamma)\, d\Omega = \mathrm{V}^* \end{aligned} \tag{1}$$

where SE is the strain energy, $\mathbf{E}$ is the constitutive elastic material property tensor, $\boldsymbol{\varepsilon}$ the strain tensor, $\mathbf{f}$ the body force per unit volume, $\mathrm{V}(\gamma)$ the volume function and V^* the given volume of material that needs to be optimally distributed in the given region Ω. The function $S(\gamma)$ denotes the material interpolation that is used to modulate the presence or absence of material using an interpolation parameter γ, which is defined below.

$$S(\gamma)=S_{\min}+\left(S_{\max}-S_{\min}\right)\gamma^{p} \qquad 0\le\gamma\le 1 \tag{2}$$

The symbol γ as defined in Eq. (2) is a spatially varying parameter that takes a value that is either zero or one to indicate the presence of absence of material respectively. In order to ease the numerical solution, this discrete optimization problem is converted to a continuous one by making γ continuously vary between zero and one. The optimization algorithm iteratively updates the value of γ at every point in the domain and drives it towards its upper and lower bounds. This is further facilitated by choosing the penalizing power p to be greater than or equal to three, which ensures that we obtain a well-defined solution [2].

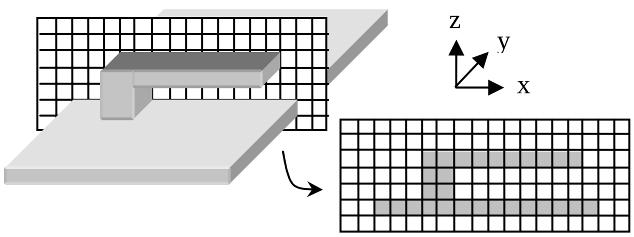

Figure 3. Vertical 2-D domains for topology optimization

Since we attempt to demonstrate how manufacturing process constraints may be imposed on the optimization algorithm, in the following treatment, we shall consider domains that are perpendicular to the substrate surface (see Fig. 3). Only two dimensional domains (i.e. extruded in the y-direction) are looked at for the sake of simplicity; however, the method may be extended to three dimensions with additional effort.

INCORPORATING MANUFACTURING CONSTRAINTS

In traditional topology optimization the presence or absence of material at any point in the domain is assumed to be independent of the state of other points in the domain. However, when manufacturing restrictions are imposed on the same problem, this assumption ceases to be valid. In the specific case of surface micromachining, deposition leads to the presence of material while etching using a mask selectively removes it in certain regions. This selective etching in a particular layer creates relief features that are propagated to the successive layers deposited above it, as explained above. When performing topology optimization under these constraints, the optimization algorithm is no longer free to choose whether to put or remove material at any point in the domain, because the manufacturing process now puts a constraint on whether or not it is possible to place material at that point in the first place. In such a situation, we readily see that the value of γ that decides the material state of a point is no longer a spatially independent parameter.

By developing the above point further, we see that, in fact, the material state of a point depends on the presence or absence of each layer below it. Different combinations of material layers produce different structures. Apart from polysilicon layers, the presence of oxide layers adds an additional complication because in the surface micromachining process, oxide layers are sacrificial in nature and are etched away in the end, leaving behind only polysilicon structures. Therefore, even

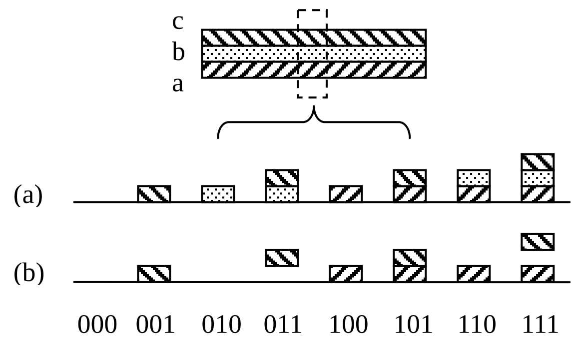

Figure 4. Eight binary combinations (binary numbers "abc") corresponding to a three layer micromachining process with oxide sandwiched between polysilicon layers (a) before sacrificial layer etch (b) after etching. Polysilicon layers are shaded differently only for clarity

though regions of oxide are not present in the final structure, they control the shape of the structure to a great deal because they determine the topology of all polysilicon layers above them.

If we define the 2D domain shown in Fig. 3 to be the x-z plane, then the surface micromachining process dictates that the material state at each point is dependent on the state of each layer below it along the z direction. If we discretize this 2D domain into rows and columns (along z and x directions respectively) as shown, then we may say that if a particular layer is absent in a column, then all layers above it in the same column move downwards by a distance equal to the thickness of this layer. In contrast, we note that there is no such dependency along the x and y directions[1]. Thus the combination of states of polysilicon and oxide layers in each column uniquely defines the material distribution in that column.

We now define an alternate set of design variables (denoted collectively as β) that correspond to the presence or

[1] In practical situations, however, this is incorrect. Due to conformal coverage of relief features (as is the case in most deposition processes), deposition of a layer causes sharp irregularities to be smoothened out along x and y directions. Hence, there is a slight dependence of material state on the state of nearby points in the *x* and *y* directions too. This too can be considered by extending the methodology presented in this paper.

absence of a particular layer in each column. The set of design variables in each column is independent from that in other columns due to independency in the x and y directions. Secondly, since the presence or absence of a particular layer in a column is not related to the state of other layers in the same column, the design variables in each column are independent of each other too. We use a value of one to indicate the presence and zero to indicate the absence of an individual layer in a column. Thus we may use this new set of independent binary design variables to reformulate the optimization problem. It is important to note these variables directly define the corresponding mask layouts. In a particular column, if the variable corresponding to a particular layer is zero it means that that corresponding etch-mask has a hole in that column.

Suppose that the surface micromachining process consists of n alternating layers of polysilicon and oxide. According to the new formulation mentioned above, every column in the domain is associated with a set of n variables that take binary values to uniquely determine the material state of all the rows in that column. Then, there are 2^n different combinations possible. This is illustrated in Fig. 4, where we consider a 3-layer micromachining process in which an oxide layer is sandwiched between a set of two polysilicon layers. The figure shows all the possible combinations of these layers in a column and their corresponding material distributions in the vertical direction.

Continuous design parameterization that intrinsically obeys manufacturing constraints

We use computationally efficient gradient-based optimization algorithms in this paper. So, in order to use solve the optimization problem involving the new binary design variables β defined in the previous section, we need to convert the discrete problem into a continuous form. This was easily achieved in the earlier formulations by continuously varying the value of γ at each point between zero and one, and then pushing the value towards the limits using a penalty term. In our formulation, due to z-dependence of the state of material, this is slightly more complicated and can be treated in the following manner.

Given an n-layer manufacturing process, each column will have to assume one among the 2^n possible configurations (denoted as Φ). We first define a basis set that has each of the 2^n combinations as members noting the fact that each of these members is linearly independent of the others. The state of each column is then defined as a linear combination of all the elements in the basis set in the following manner.

$$C_i = \sum_{j=1}^{2^n} \Phi_j \cdot c_{ji}\left(\beta\right) \tag{3}$$

The quantity Φ_j represents the j^{th} binary combination in the basis set and c_{ji} is the coefficient of this combination in the expression for the i^{th} column. Each Φ_j is associated with a unique n-digit binary number that defines the presence or absence of a layer in that combination. The coefficients are functions of the design variables (β) and are chosen in such a manner that for a given combination of $\beta_i s$ in a column, only one of the coefficients will assume unit value while the rest will be zero. This ensures that for a given combination of $\beta_i s$, the state of a column will correspond to one and only one of the elements in the basis set. This is done by defining the coefficients in terms of the design variables as follows.

$$c_{ji}\left(\beta\right) = f_j\left(\beta_{i1}\right) \times f_j\left(\beta_{i2}\right) \times \cdots \times f_j\left(\beta_{in}\right)$$

$$f_j\left(\beta_{ik}\right) = \begin{cases} \beta_{ik} & \text{if the } k^{th} \text{ layer is present in } \Phi_j \\ 1-\beta_{ik} & \text{if the } k^{th} \text{ layer is absent in } \Phi_j \end{cases} \tag{4}$$

It is easy to verify that for any combination Φ_j, c_{ji} is unity only when all the $\beta_i s$ are identical to the digits of the n-digit binary number associated with Φ_j.

With the help of the above modeling, we now proceed towards the continuous optimization problem. If the $\beta_i s$ take values in between zero and one, the coefficients will not have integer values; instead they will all assume fractional values between zero and one. This means that the state of the i^{th} column will not correspond to a single one of the combinations but will be a weighted sum of all the combinations. The column will achieve the pure state only when all the $\beta_i s$ go either to zero or to one. Thus we relate the state of the column to the design variables that are associated with that column in a continuous manner.

The above process is done in a similar manner for each column in the domain. Each column has a set of associated $\beta_i s$, which are used to calculate the coefficient values corresponding to that column. This is stored as a matrix, which is referred to as the "*coefficient matrix*" C, whose elements c_{ji} are the same as those defined in Eqs. (3) and (4).

The original optimization problem stated in Eq. (1) was defined in terms of the material interpolation parameter γ. Since we are now defining a new set of design variables, we have to find a method of relating γ to β so that Eq. (1) may be rewritten in terms of the new design variables. In order to do this, we go back to Eq. (3) to give it more mathematical significance. The quantity Φ is just a symbol that represents a particular combination in the basis set. However, given any such columnar combination, we can readily work out the distribution of material in each row of that column. Thus, knowing the binary combination (Φ) corresponding to each column in the domain, we can deduce γ_{ij}, the value of γ in the i^{th} row of the j^{th} column in the domain.

We formally define this as the "*material distribution matrix*" D. For any column, the elements of the material distribution matrix d_{ij} are defined as one if the i^{th} row of the j^{th} combination in the basis set has polysilicon (i.e. a material state of unity) and zero if it is void (i.e. a null material state). Knowing the associated binary combination for each column, the exact material distribution in the rows of that column can thus be determined.

To sum up these results mathematically, the coefficient matrix and material distribution matrix can be used to relate the new design variables β to the material interpolation parameter γ as follows.

$$\gamma_{ij} = \sum_{k=1}^{2^n} d_{ik} \cdot c_{kj}\left(\beta\right) \quad (5)$$

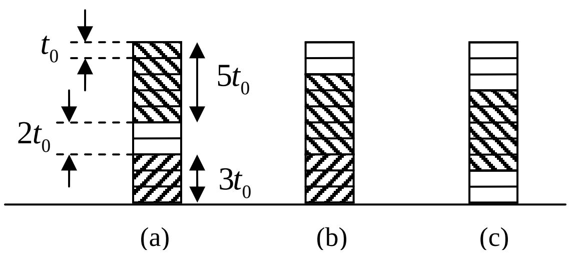

Figure 5. Discretization of a column into rows such that each layer is an integral multiple of the unit thickness for (a) “111”, (b) “101” and (c) “011” configurations.

It is interesting to note the similarity between Eq. (3) and Eq. (5). In fact, they are both statements of the same idea in different forms. Every column C_i in Eq. (3) has now been discretized in the vertical direction into a number of rows and Eq. (5) gives the material state of a particular row of this column. This column may have any one of the 2^n binary combinations, but if the β values associated with that column are either zero or one, then only one of the 2^n coefficients will be active. This means that only that particular d_{ik} will get selected. For β values between zero and one, the resulting γ values will be “grayed-out” and will no longer be purely black or white. The role of the optimization algorithm is to take β values to their appropriate limits, thereby yielding a converged (black and white) solution.

One additional point that remains to be emphasized here is the difference between material layers and the rows mentioned above. Every surface micromachining process involves deposition of several layers of different thicknesses. When a particular material is selectively etched away in a certain region, it causes the layers above it to be deposited at a lower height (i.e. lowered by a distance equal to the thickness of the layer). During the course of optimization, the algorithm must have the freedom to switch each layer on and off (i.e. vary the corresponding value of β between zero and one) selectively in certain regions. However, the movement of material layers due to this switching will mean that the finite element mesh that discretizes the domain should be re-done in order to capture this movement. This violates the basic tenet of any topology optimization routine, according to which the domain and the finite element mesh do not change from one iteration to the next.

We resolve the above conflict by using a different procedure in which although the material distribution within the domain changes due to switching of layers, the actual finite element mesh remains fixed. In order to do this, we define a unit thickness such that the thicknesses of each layer in the micromachining process can be expressed as an integral multiple of this unit thickness. In other words, if the thickness of each layer is represented as t_i, then the unit thickness t_0 is such that t_i/t_0 is an integer for all $1 \le i \le \mathrm{n}$. Thus, t_0 is the greatest common divisor of all t_is. If we now discretize the layers into rows in terms of this unit thickness, then we see that every layer occupies an integral number of units or rows (see Fig. 5).

In the absence of a particular layer, the layers above it now move by integral multiples of the unit thickness (since the thickness of each layer is ensured to be a multiple of the unit thickness). This ensures that the each layer always occupies an integral number of rows irrespective of the presence or absence of other layers. If we choose the finite element mesh to coincide with this discretization of rows, then from Fig. 5, we see that although the material properties of mesh elements change due to the switching of layers, the mesh geometry itself does not have to change in order to accommodate this switching. This enables us to have a fixed finite element mesh in order to perform the topology optimization.

Sensitivity Analysis

Having defined a set of design variables that enable continuous distribution of material even in the presence of manufacturing constraints, the next step is to derive the formulas for the sensitivity of the objective function in Eq. (1) with respect to each of these design variables. This analysis is used in the optimization algorithm to update the design variables during each iteration step. In traditional topology optimization, sensitivity analysis is performed with respect to the original set of design variables γ. In our new formulation, we differentiate Eq. (5) partially with respect to β and substitute this into the expression for sensitivities with respect to γ in order to get the sensitivities with respect to the new design variables.

$$\frac{\partial\phi}{\partial\beta_{ij}} = \frac{\partial\phi}{\partial\gamma_{kj}} \times \frac{\partial\gamma_{kj}}{\partial\beta_{ij}} = \frac{\partial\phi}{\partial\gamma_{kj}} \times \left(d_{kl} \frac{\partial c_{lj}}{\partial\beta_{ij}} \right)$$
$$1 \le i \le n, \quad 1 \le j \le n_c \quad (6)$$
$$1 \le k \le n_r, \quad 1 \le l \le 2^n$$

Here ϕ is the objective function (strain energy in this paper), n is the number of layers in the manufacturing process, n_c is the number of columns and n_r is the number of rows (which is equal to the sum of number of units that discretize the individual layers).

NUMERICAL IMPLEMENTATION

We implemented the numerical scheme for performing topology optimization with manufacturing constraints using the COMSOL Multiphysics® platform [17]. We used the COMSOL scripting language to write the code. The COMSOL scripting language is very similar to MATLAB programming language and allows user defined functions to be incorporated along with its finite element analysis functions. We made use of this feature to create a generic set of functions that can handle any arbitrary surface micromachining process. Given the constitution and thickness of each material layer in the fabrication procedure, we can thus generate optimal topologies under the imposed manufacturing constraints.

We used the optimality criteria method to solve the topology optimization problem. The algorithm was implemented along with a mesh independency filter in order to avoid checkerboard patterns in the final solutions [18].

The formulation was tested using examples where optimized topologies that were manufacturable in the PolyMUMPS® process [15] were sought. The PolyMUMPS® process is an industry standard for surface micromachining process flows. It is a five layer process that consists of three polysilicon layers and two silicon oxide layers deposited in an alternating manner. The thickness of each of these layers is given in Table 1.

Table 1: Material layers that comprise the PolyMUMPS® microfabrication process. Layers are numbered starting from the lowest layer that is also the one deposited first.

Layer	Material	Thickness (µm)
1	Polysilicon (P0)	0.5
2	Silicon Oxide (O1)	2
3	Polysilicon (P1)	2
4	Silicon Oxide (O2)	0.75
5	Polysilicon (P2)	1.5

In the numerical examples presented in this paper, we have assumed that the lowest polysilicon layer (P0) is not constrained in any way apart from the boundary conditions defined in the problem. In other words, we do not assume that P0 is deposited on some substrate surface and is therefore fixed to the substrate. This assumption assures that the bottom edge of the domain is not unnecessarily constrained. In practice, this may be realized by etching the substrate under this part to create an over-hanging structure. The main reason for this assumption is that we have chosen two benchmark problems in topology optimization to show how the optimal topologies that obey manufacturing restrictions compare with those that do not obey. For examples where the entire bottom edge is fixed, this restriction does not apply and those examples will be realistic for microsystems. Thus, it should be noted that the examples included below are in no way restrictive to apply the methodology of this paper for realistic situations.

RESULTS

The new formulation was used to solve the problem of finding the optimal topology for a cantilever that is loaded at the free end. This is a benchmark problem for topology solution. The design domain and the boundary conditions are shown in Fig. 6. The resulting optimal topology is shown in Fig. 7 along with the mask layouts corresponding to each of the layers.

We also applied the method to solve the MBB-beam (another benchmark) problem [2] for a beam supported at both ends and bearing a vertical load in the middle. We modeled half the beam, applying symmetry boundary conditions as shown in Fig. 8.

In both the examples, it was observed that the optimal topologies resemble their unconstrained (i.e., without the

Figure 6. Design domain for the cantilever problem with boundary conditions

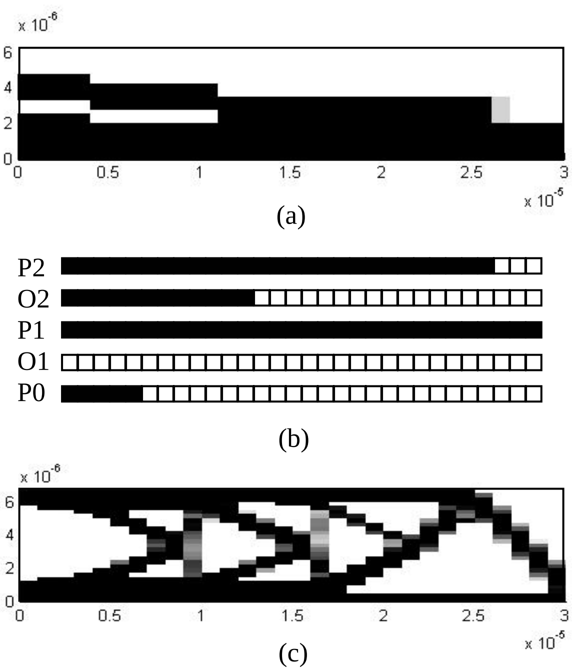

Figure 7. Optimal solution for the cantilever problem (a) Resulting topology (Strain Energy = 3.9414e+9 Joules) (b) Corresponding mask layout (c) Optimal topology generated without surface micromachining constraints (Strain Energy = 1.4189e+9 Joules)

manufacturing restrictions) topologies shown. These correspond quite well with the results found widely in the literature. Any changes discerned are direct consequences of the imposition of the manufacturing constraints. It is seen that the strain energies of the new topologies are of the same order of magnitude as the original ones but are higher. This indicates that the new topologies are optimal, but only in the new design space. Clearly, the restrictions of surface micromachining do not allow features that are inclined or curved. Hence, only stepped features that are all too common in surface micromachining are obtained. So, truly optimal topology is not possible. Thus, we show the compromise in performance (in this case, the strain energy) due to manufacturing constraints. Slight gray areas around the edges are not uncommon in optimal topologies. A noteworthy feature, however, is that gray vertical strips occur due to columnar nature of design parameterization used in this paper. With finer discretization, such artifacts may be minimized.

Our ongoing work is focused on applying the new design parameterization scheme to microsystem problems of relevance. These include electrostatically or electro-thermally actuated structures and compliant mechanisms. Extending this approach to two directions to realize a 3-D design is also a part of future work.

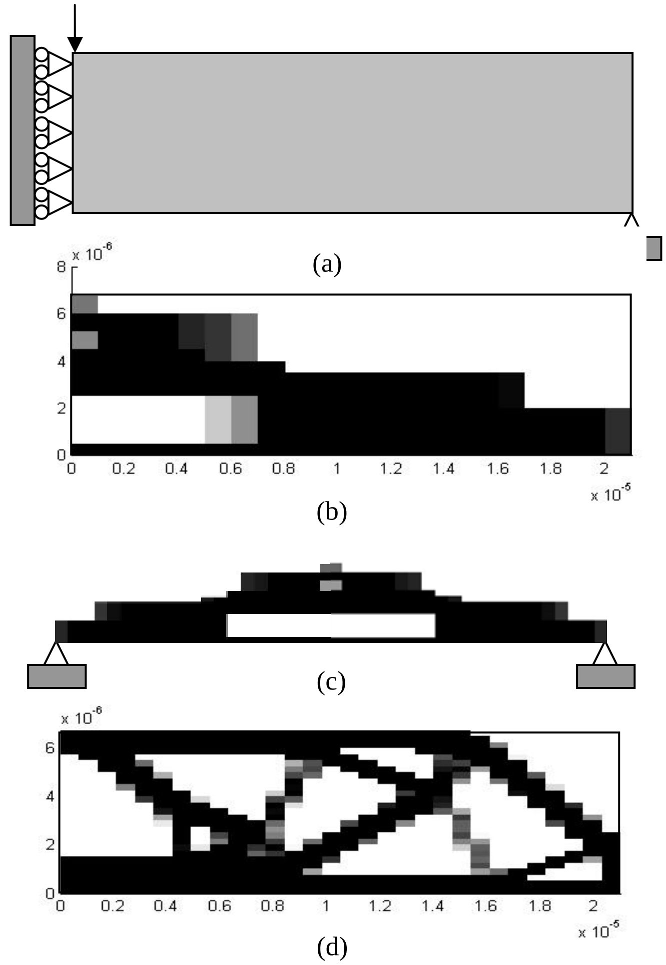

Figure 8. Topology optimization of the MBB-beam. (a) Half design domain with symmetry boundary conditions (b) Resulting topology (Strain Energy = 1.4916e+9 Joules) (c) Entire MBB-beam (d) Optimal topology generated without surface micromachining constraints (Strain Energy = 0.58882e+9 Joules)

CLOSURE

Topology optimization has been applied to a wide variety of problems at the macro and micro scale systems. To increase its applicability and usage further, it is important to incorporate manufacturing restrictions. In this paper, by focusing on surface micromachined micromechanical structures, a novel continuous design parameterization for incorporating the limiting features of layered surface micromachining process is presented. The new method can deal with any number of structural and sacrificial layers of varying thicknesses in a process. The finite element mesh remains fixed as in all topology optimization problems. A novel feature of the design parameterization presented here is that the design variables that determine the optimal material distribution collectively change the formation of each vertical column in a 2-D vertical cross-section. The modeling is simple enough to be able to directly implement on commercial software platform of COMSOL MultiPhysics®. This naturally implies that we can solve a wide variety of problems in the future by paying due attention to manufacturing constraints of the micro-scale processes. Extensions to macro manufacturing are also not precluded by the novel approach to material distribution over a fixed reference domain.

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