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14. ABSTRACT

We developed, implemented, and validated new topology optimization strategies/algorithms for the design of microelectromechanical systems (MEMS) exhibiting coupled multiphysics behavior. The numerical tools include a fully coupled nonlinear electro-thermo-mechanical and electrostatic-mechanical finite element solvers, and novel sensitivity analysis modules that allow the evaluation of the gradients of the coupled response with respect to a large number of optimization variables. These tools have been integrated into the overall topology optimization design environment.

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TOPOLOGY OPTIMIZATION FOR THE DESIGN OF 3-D MICROELECTROMECHANICAL SYSTEMS (MEMS) UNDERGOING COUPLED MULTIPHYSICS PHENOMENA

AFOSR F49620-02-1-0037

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Overview

During the three years of this exciting research program, we developed, implemented, and validated new topology optimization strategies/algorithms for the design of microelectromechanical systems (MEMS) exhibiting coupled multiphysics behavior. Underpinning our research is the realization that a large class of MEMS fabrication technologies, for example, bulk and surface micromachining, are now quite mature as evidenced by the number of commercial foundry services available. The stability of this fabrication infrastructure is such that structural innovations can proceed not only in a heuristic manner, but also via systematic design approaches. The development of such design approaches was the overarching objective of this research. Potential Air Force applications that can be impacted by our design technology are numerous and include actuators/switches for optical and RF communications, microsensors, and micromachined fans/turbines for microcooling, mixing, and even power generation.

Topology optimization provides a tool to tailor the distribution of the constituent materials, within an individual layer and through the thickness of many layers, to create structures and devices that perform in a desired manner. We have successfully developed novel topology optimization technology for micro/nanosystems devices that experience multiphysics phenomena, validated it experimentally where possible, and implemented it into a computational design environment. The numerical tools include a fully coupled nonlinear electro-thermo-mechanical and electrostatic-mechanical finite element solvers, and novel sensitivity analysis modules that allow the evaluation of the gradients of the coupled response with respect to a large number of optimization variables. These tools have been integrated into the overall topology optimization design environment. Our overall computational design and analysis environment is demonstrated in Fig. 1. Three broad classes of problems that represent applications across a wide cross-section of micro and nanosystems technology have driven our efforts; each are described in the following sections.

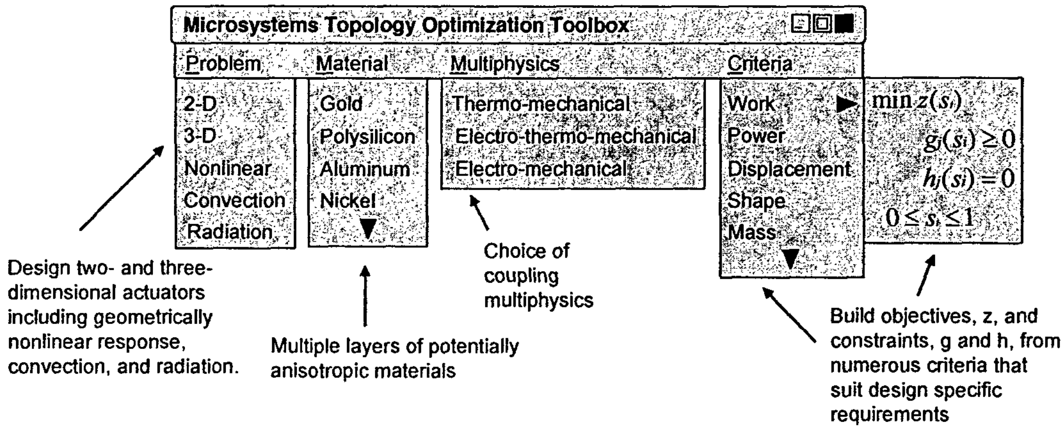

Fig. 1 Illustration of the overall computational design environment that illustrates the capabilities of our approach.

Actuation via Misfit Strains

In this class of problems misfit strains, for example thermal expansion mismatch between the constituent materials in a thin-film structure lead to deformation. If the deformation is blocked, a useful actuation force can be obtained. Furthermore, this strategy can be used to fabricate devices that have three-dimensional features from a standard two-dimensional microfabrication process! In addition to thermal expansion mismatch, the approach is applicable to other sources of misfit strains, e.g., piezoelectric, shape memory, and embedded pneumatic/hydraulic actuation. In this class of problems there is a *one-way coupling between thermal and mechanical phenomena.* Figure 2 illustrates our general capabilities here.

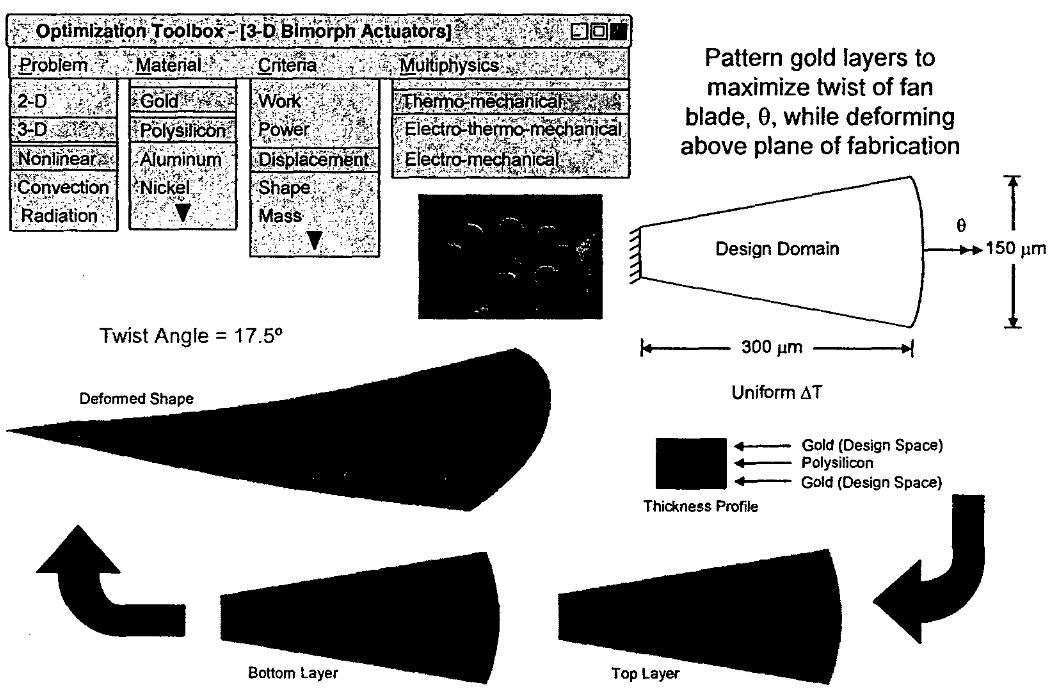

Fig. 2 Illustration of the thermomechanical capabilities in our topology optimization toolbox.

An example is shown in Fig. 3 where the goal is to design a micro "screwdriver" that undergoes a desired twist along the right edge of the design domain while the left edge is clamped. The design domain contains a fixed layer of polysilicon sandwiched between two outer layers of gold, which can be arbitrarily patterned. With respect to the deposition temperature, the design domain is uniformly heated to yield deformation. Figures 3(a) and 3(b) show the optimized layouts of the upper and lower gold layers (red = gold, blue = polysilicon). The strips near the constrained edge provide the twisting moment, which is accentuated by the crossing pattern of the upper and lower gold layers along the length. The deformed shape is depicted in Fig. 3(c) where the screwdriver is viewed along the twist axis looking from the unconstrained edge.

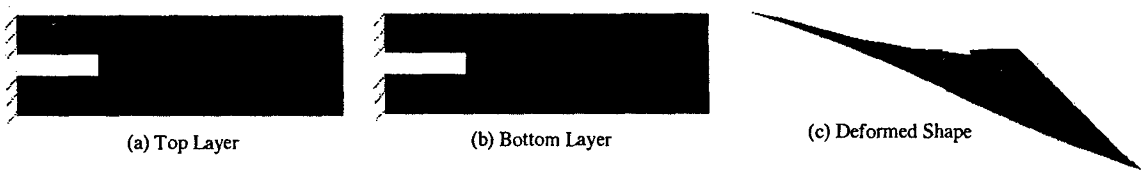

Fig. 3 Optimal layout (a) and (b) of the patterned multilayer structure designed to yield a prescribed angle of twist upon heating (or more generally, via misfit strains between the layers). This example demonstrates the complex interaction of coupled thermo-mechanical phenomena incorporating geometrically nonlinear deformations; (c) shows the deformed shape, looking along the structure twist axis.

Figure 4 shows results of a similar problem where a cantilevered plate is designed to curve as much as possible along its length, while minimizing the transverse curvature of the free edge (keeping it as flat as possible). This problem is motivated by applications in microfluidic mixing. Curvature results from thermal expansion mismatch between two thin film layers (gold and polysilicon). If the cantilevered structure consisted of a polysilicon plate fully covered by a gold film, significant biaxial curvature would occur which detracts form device performance. Figure 4(a) shows optimally-designed thin-film structures that we fabricated and tested; Fig. 4(b) shows predicted and measured displacements along the free edge of the 300 μm x 300 μm plate. The agreement is excellent, especially considering that the measured and predicted deflections across the free edge are on the order of 0.1 μm while the total deflection of the free edge is about 30 μm!

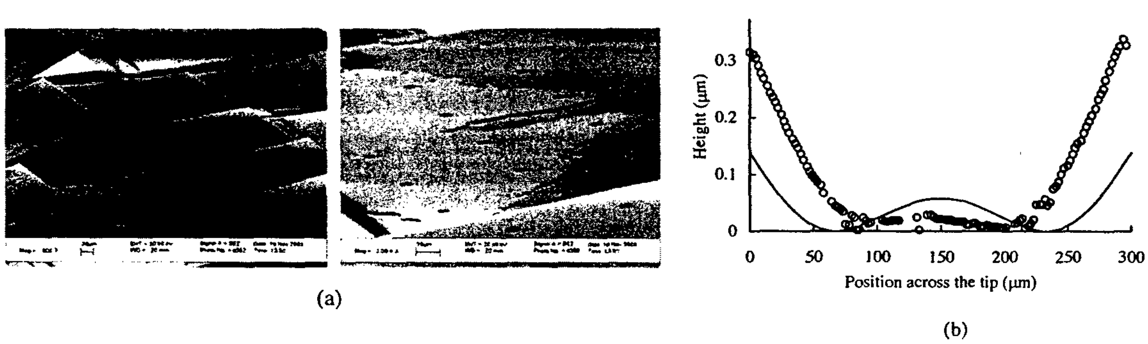

Fig. 4 (A) Fabricated samples of optimally-designed gold/polysilicon multilayer plates – the one on the right is 300 x 300 μm with a 1.5 μm thick polysilicon plate covered by a 0.5 μm thick patterned gold film; (b) measurements and predictions of the deflection across the free edge of the plate.

Electrothermomechanical Actuation

In this class of problems misfit strains are generated electrothermally. An applied electric potential leads to current flow, which results in a nonuniform temperature distribution via Joule heating, which then results in strain. There is essentially a *one-way coupling between electrical, thermal, and mechanical phenomena.* Figure 5 illustrates our general capabilities here.

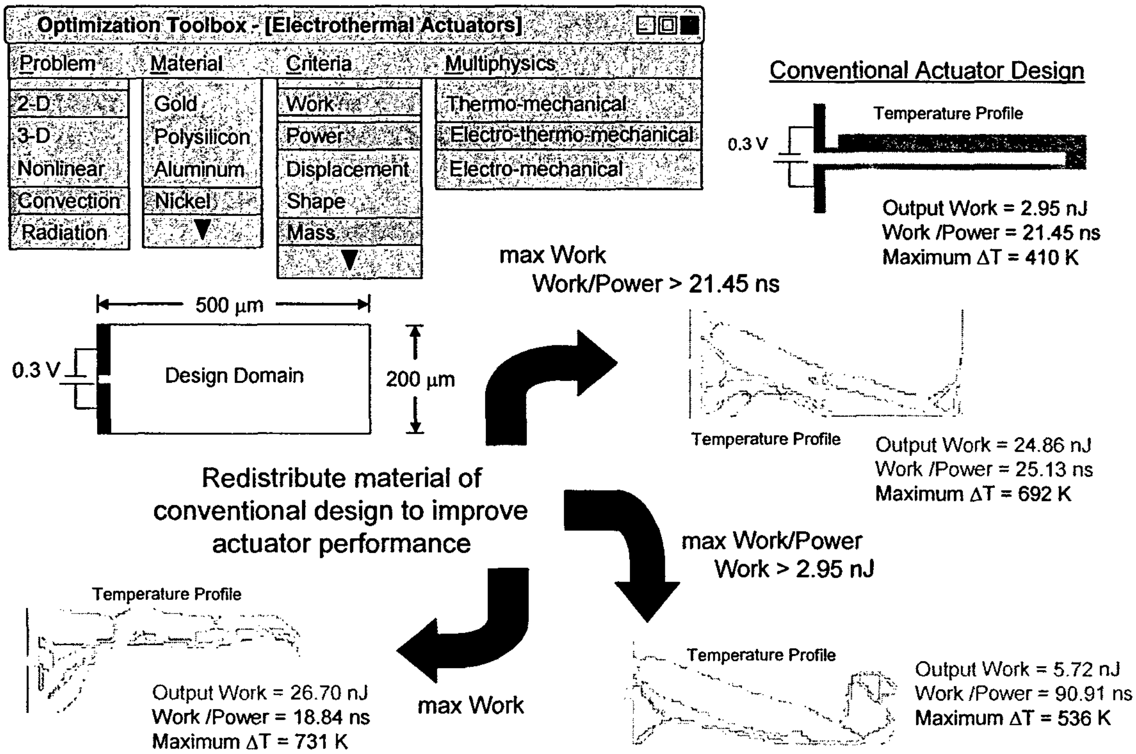

Fig. 5 Illustration of the electrothermomechanical capabilities in our topology optimization toolbox.

In Fig. 6, electrothermal Joule heating is used to heat the device and thus cause deformation or generate force. In this case electro-thermal-mechanical coupling is considered in the design process. The objective is to find the geometry of the polysilicon device that maximizes the vertical displacement of the midpoint along the right edge, while restricting its maximum mass. External loads are represented by a spring attached to the midpoint. As shown in Figure 3(a), two electrodes are attached along the left edge of the domain. These ports also serve as mechanical supports. Using a novel multi-physics material interpolation scheme in the topology optimization process, the optimal geometry and resulting temperature distribution shown in Figure 3(b) is generated, and the deformed structure is depicted in Figure 3(c). The optimized structure generates heat by creating a short connection between the electrodes, which maximizes the Joule heating in this area. The expansion of the thin lower arm from the temperature increase provides the push to lift up on the opposite edge. The optimized result produces over twice the displacement as compared to conventional beam-type electrothermal actuator designs!

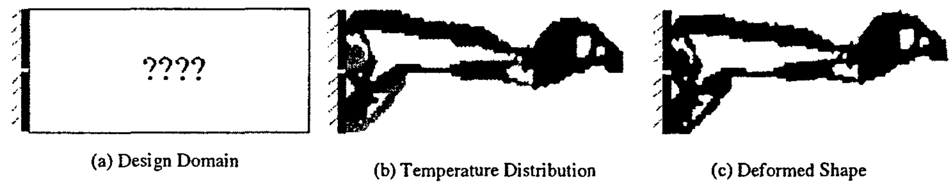

Fig. 6 (a) Design domain; and (b), (c) optimal material layout for an electro-thermo-mechanical actuator; (b) shows the nonuniform temperature distribution through the actuator upon application of an electrical potential, and (c) shows the resulting deformed shape. This example demonstrates the complex interaction of coupled electro-thermo-mechanical phenomena incorporating geometrically nonlinear deformations.

Here we couple the in-plane electrothermal behavior just described with out-of-plane actuation as shown in Fig. 7. This is done by fabricating the device using a gold/polysilicon bilayer film with structurally constrained electrodes held at a potential difference of 1 V, and at the temperature at which convection with the surroundings does not take place on opposite sides of the design space. The objective is to maximize the vertical out-of-plane displacement along the midpoint of one edge as shown in Fig. 7 by appropriately patterning the gold/polysilicon bilayer, which is constrained to occupy 50% of the full design space. The optimal distribution patterns along with the resulting temperature and voltage distributions in the body are shown in Fig. 7. The structure deflects 6 μm out of the plane and Fig. 7 also shows the deformed configuration. The optimal structure operates by the creation of a significant temperature increase in the center member that via the gold/polysilicon bilayer results in the bending moment responsible for the upward push.

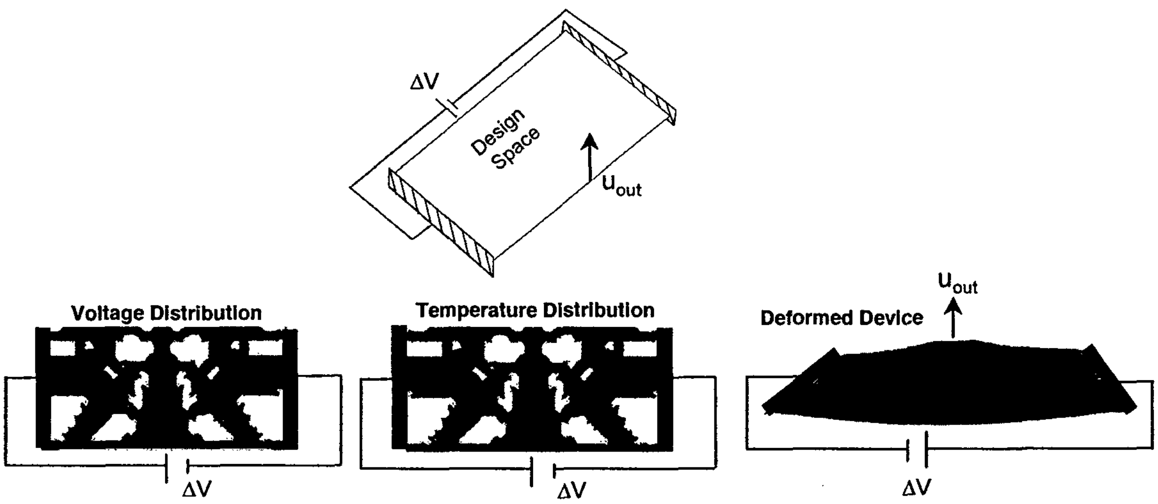

Fig. 7 200 by 100 μm design space for a gold/polysilicon electro-thermo-mechanical actuator designed to deflect out of the plane of the 2-D geometry. The optimal topology is shown in the three figures across the bottom; in the first two white space denotes voided regions while in the third blue denotes void and red denotes bilayer material. From left to right, the voltage and temperature distributions (red is high, blue is low) are shown, along with the deformed shape.

Electrostatic-Mechanical Actuation

Here an applied potential across conductors leads to a generally nonuniform electric field between them, which results in an electrostatic force which deforms the conductors. As the conductors deforms the electric field changes, which in turn changes the force, and so on. As a result, *there is full coupling (two-way) between electrical and mechanical phenomena.* The full coupling between the electrostatic and mechanical fields significantly increases the complexity of the formulation and solution of the corresponding topology optimization problem. Figure 8 illustrates our general capabilities for this class of problems.

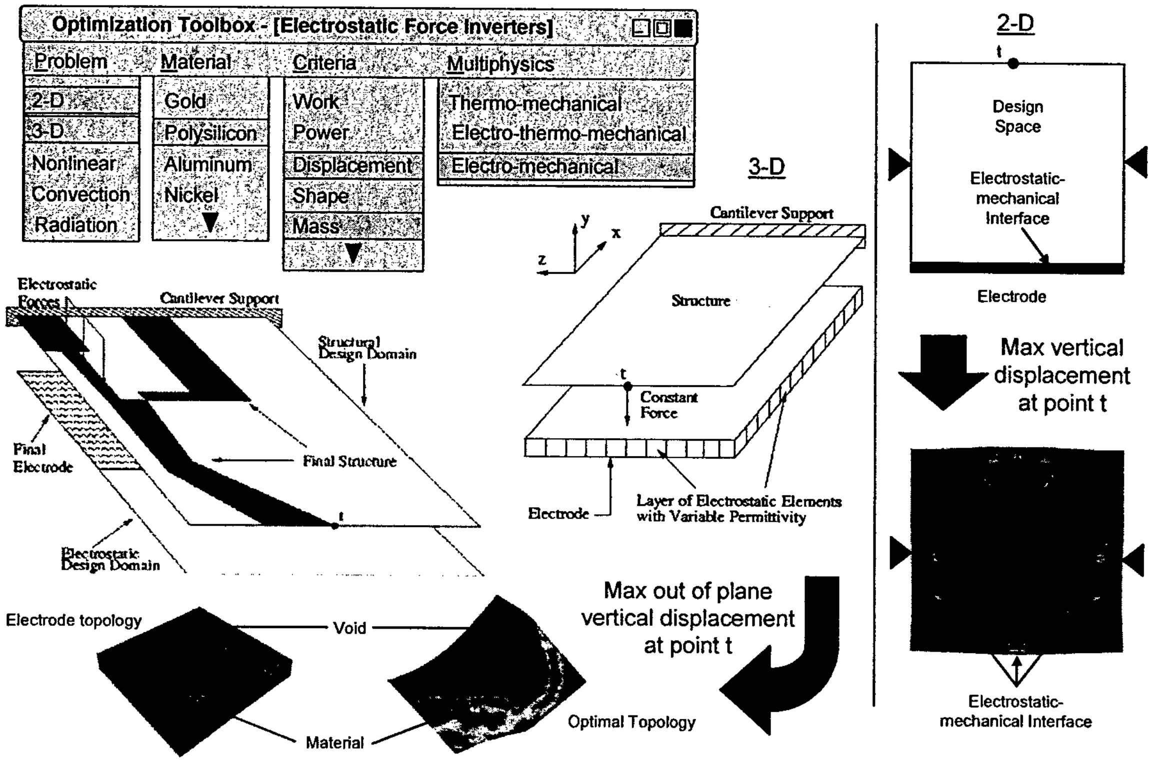

Fig. 8 Illustration of the electrostatic-mechanical capabilities in our topology optimization toolbox.

In Fig. 9 we consider the design of an electrostatically actuated force-inverting mechanism. An electrode is attached to the lower edge of the design domain, and two electrical ports are positioned at the center of the vertical edges, which also serve as mechanical supports. The optimization problem is subject to a mass constraint and a strain energy constraint that indirectly prevents the mechanism from being electrostatically pulled-in. Two cases are compared: i) the electrostatic/mechanical interface is fixed and cannot be varied in the optimization process, and ii) the geometry of the interface can evolve in the optimization process. The optimized density distributions for both cases are shown in Figs. 9 b and c. In the case of a fixed interface, all material is needed to withstand the large electrostatic pressure and to prevent the mechanism from pull-in. Only a minor lifting force at point "C" is generated. In contrast, a *novel free interface feature developed under this grant* allows removing material close to the electrode and generating a structural design that yields a significant lift-up at point "C". The actuated, deformed structure is shown in Figure 9c.

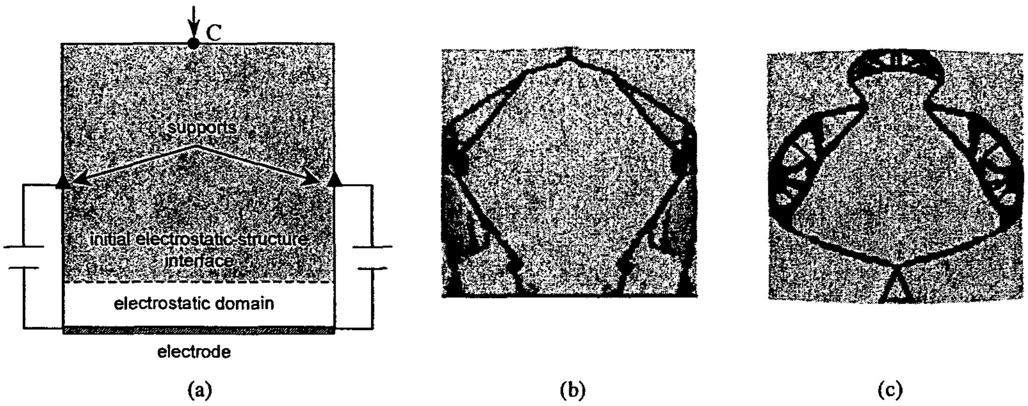

Fig. 9 (a) Design domain for the electrostatically-actuated force inverting mechanism, along with the optimum designs for the cases where the electrostatic-structure interface is (b) fixed, and (c) free.

Our final example extends the capabilities demonstrated in the precious two-dimensional example to a full three-dimensional situation. The design problem is depicted in Fig. 10a. The problem is to find a plate structure that when subjected to electrostatic forces lifts up point "*t*" which is subject to a given force acting downwards. The design problem is subject to a constraint on the mass and upper and lower constraints on the strain energy. The energy constraints are needed to avoid instabilities and, at the same time, to favor a flexible design. In this example, *the topology of the structure and the electrode are simultaneously optimized.* This unique and novel feature allows for additional improvement in performance.

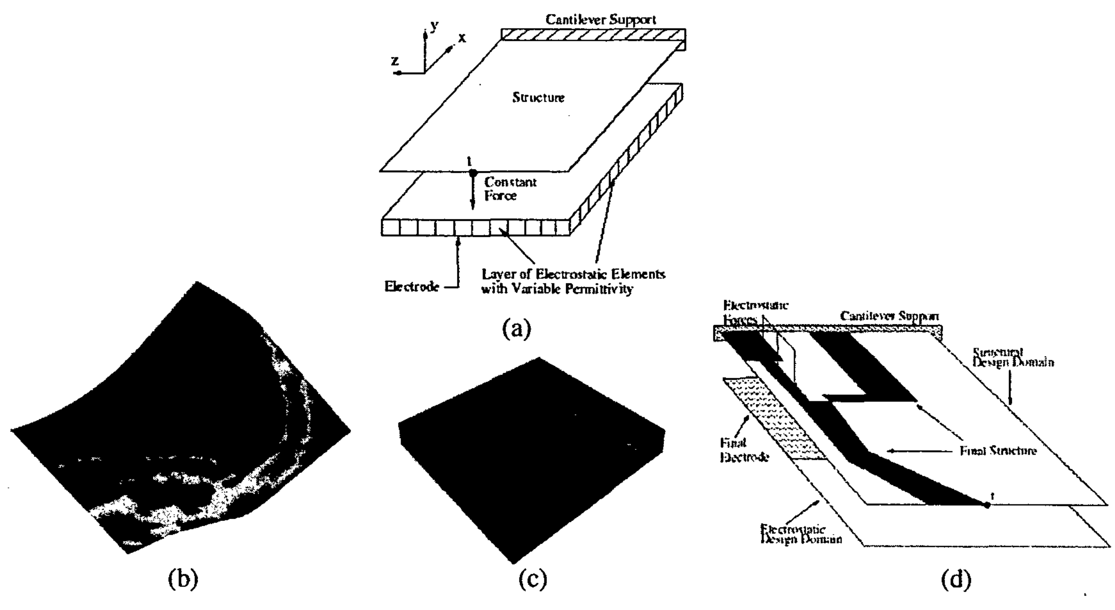

Fig. 10 (a) Design problem for the 3-D electrostatically-actuated mechanism, along with (a) the optimized material distribution in the deformed configuration, (b) the optimized electrode topology, and (c) a schematic illustrating the way the optimized design works.

The material distribution in the deformed configuration is shown in Fig. 10b. The optimized topology of the electrode is shown in Fig. 10c. Based on these results a conceptual design has been created which is shown in Fig.10d. The schematic illustrates the actuation mechanism: the center part of the device, connected to the support, serves as a fulcrum. The part of the device attached to the side of the support is pulled downward by the electrostatic forces, allowing the curved lever arm (connected to node '*t*') to rotate around the center support. It is noteworthy that the optimizer could not find a design that lifts-up point "*t*" without optimizing simultaneously the geometry of the electrode.

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