Topology optimization of self-sensing nanocomposite structures with designed boundary conditions

Ryan Seifert1, Mayuresh Patil and Gary Seidel1

460 Old Turner St, Blacksburg, VA 24060, United States of America

E-mail: rseifert@vt.edu, mpatil@vt.edu and gary.seidel@vt.edu

Received 31 January 2019, revised 14 March 2019
Accepted for publication 20 March 2019
Published 6 June 2019

Abstract
Controlling volume fractions of nanoparticles in a matrix can have a substantial influence on composite performance. This paper presents a topology optimization algorithm that designs nanocomposite structures for objectives pertaining to stiffness and strain sensing. Local effective properties are obtained by controlling local volume fractions of carbon nanotubes (CNTs) in an epoxy matrix, which are assumed to be well dispersed and randomly oriented. The method is applied to the optimization of a plate with a hole structure. Several different allowable CNT volume fraction constraints are examined, and the results show a tradeoff in preferred CNT distributions for the two objectives. It is hypothesized that the electrode location plays an important role in the strain sensing performance, and a surrogate model is developed to incorporate the electrode boundary as a set of additional design variables. It is shown that optimizing the topology and boundary electrode location together leads to further improvements in resistance change.

Keywords: topology optimization, multifunctional optimization, nanocomposites, boundary condition optimization, strain sensing

(Some figures may appear in colour only in the online journal)

1. Introduction

Recent developments in advanced materials have led to the emergence of multifunctional structures that ‘combine the functional capabilities of one or more subsystems with that of the load bearing structure’ [1]. One of these capabilities is self-sensing, in which a structure is able to directly collect information about its operating environment and relay that information to pilots, testing engineers, and maintenance engineers [2, 3].

The inability to embed a traditional sensor (such as a strain gauge) in the structure is a significant limitation for composites, in which cross-sectional or interlaminate failures may not be observable at the surface [4]. This motivates the investigation of multifunctional structures in which the sensing material is dispersed throughout the structure. Of course, this sensing structure must still perform its role as a load carrying member. Of the candidate materials for use in creating self-sensing structures, carbon nanotubes (CNTs) are the subject of much attention [5]. CNT based composite strain sensors have been shown to have higher sensitivities than classic strain gauges at the macroscale [6] and exhibit strain sensing through several mechanisms [7].

Paralleling the rise in multifunctional materials is the blooming field of additive manufacturing. Specifically, composite additive manufacturing continues to be a hot topic in labs, where ‘Additive manufacturing holds strong potential for the formation of a new class of multifunctional nanocomposites through embedding of nanomaterials [8].’ It is even possible to additively manufacture CNT/polymer composites with finely tailored microstructures using liquid deposition [9].

Recently, much has been done to apply topology optimization to the design of multifunctional materials. Maute et al [10]
used level set topology optimization to design a set of printable shape memory polymer (SMP)-elastic matrix composites to match a specified deformed shape once actuated. This two-material system was able to closely match a deformed shape once actuated, and showed that there is indeed benefit to combining advanced manufacturing, multifunctional materials, and topology optimization. Pertaining more specifically to sensing structures in topology optimization, Rubio [11] investigated topology optimization of a piezoresistive patch in a compliant mechanism in which orientation of a monolithic Wheatstone bridge was optimized in addition to the topology of the compliant structure. Gusti, Mello, and Silva [12, 13] optimized the topology of a piezoresistive membrane that was stretched over a structure to maximize the sensing capability and the stiffness. They were able to show over 150% increases in measured potential difference due to the piezoresistive effect.

However, a limitation of most published work is the focus single or two-material systems. Given the advances in additive manufacturing, it is possible to envision a finely controlled structural system with a locally varying, or graded microstructure. This paper presents an algorithm capable of designing such a structure. This is done via an application of topology optimization, in which the design variables are set to be the local CNT volume fractions of a CNT/Epoxy composite structure and the objectives are measures of structural stiffness and electrical resistance change due to strain (strain-sensing).

A plate with a hole, loaded in tension in the vertical direction, is selected as the test structure. Constraints are imposed on both the local and global CNT volume fractions as representations of manufacturing and cost constraints, respectively. Micromechanics models are used to obtain element effective properties and are functions of the local CNT volume fraction, and finite element analysis uses these local effective properties to solve for the global objectives. Sensitivities of the objectives are analytically derived and used to fuel a gradient-based, Sequential Quadratic Programming (SQP) optimization scheme.

It has also been seen that the simultaneous optimization of sensor and structure can highly depend on the selection of the electrode location [14]. While a structural loading environment is often not at the discretion of the engineer to prescribe, it is much more likely that one may choose where to locate the electrodes on a structure, and in doing so may improve sensing or decouple the trade-off between stiffness and sensing.

The test structure is first optimized with a set of fixed electrodes. Then a surrogate model is developed to incorporate the discrete electrode variables (start and end nodes within a FEA mesh) within the continuous optimization scheme.

Section 2 details the problem statement, design space, and solution algorithm. Section 3 follows with the relevant micromechanics, finite element equations, and sensitivities of the objectives. Section 4 presents results for the optimization of the fixed-electrode structure, commenting on differences in performance for various volume fraction constraints as well as interpreting what makes designs optimal in one or multiple objectives. Section 5 introduces the boundary condition surrogate model and relevant equations and sensitivities. Section 6 then solves the combined topology and boundary condition optimization problem and compares the results to the fixed-electrode case. Conclusions are presented in section 7.

2. Problem statement

Topology optimization seeks to design a structure by first discretizing the design space and then driving the local material volume fractions in each element of that space to their optimal values. The general problem is formulated as follows:

\[
\min F(\nu) = F(f_1(\nu), f_2(\nu)) \\
\text{s.t. } 0 \leq \nu_e \leq 1 \\
\sum \nu_e \leq V_p
\]  

Here the set of design variables are designated as the vector \( \nu \), and may correspond to a ‘relative density’ of material or a phase volume fraction. The relative density in each element is denoted by \( \nu_e \). The objective function \( F(\nu) \) may be multibjective, and be formed from single objective functions \( f_1 \) and \( f_2 \). For this paper \( f_1 = \Delta R(\nu)/R_0(\nu) \), the resistance change due to strain, and \( f_2 = U(\nu) \), the strain energy. In pseudo-density methods such as SIMP or RAMP [15] the design variables are used within one or more material interpolation schemes, which govern the effective material properties of the corresponding element. It is the aim of the optimization to find the set of \( \nu \) that minimize the objectives. Classically these methods include some penalty term that drives \( \nu_e \) to either 0 or 1, representing either material or void. For more detailed reviews of topology optimization the reader is encouraged to examine [15] and [16].

Rather than considering a single material property and driving this property to 1 (on) or 0 (off) via a SIMP-like method, one may instead consider a micromechanics model, such as a rule of mixtures [17, 18], inverse rule of mixtures [17, 19], or a method that makes use of the Eshelby solution [20], such as the Mori-Tanaka method [21]. These models relate effective material properties to the volume fraction of an inhomogeneity in a matrix in a continuous manner. In the case of this paper, that inhomogeneity is the volume fraction of randomly oriented and well-dispersed CNT in each element. As no artificial penalization is added, what results is no longer an ‘on’ or ‘off’ design, but rather a distributed system of CNT-epoxy nanocomposite in which each element may have a different material composition, and different effective properties.

The design space for the plate with a hole is introduced in figure 1, making note of symmetry boundary conditions that are used to reduce the design space to a single quadrant. The left and bottom edge contain this symmetry condition, the top edge is loaded with a uniform tensile load, and the blue and red lines mark the locations of the electrodes. Constraints are placed on both the amount of CNT available to a single element and on the total amount of CNT in the cross-section; \( V_p \) and \( V_{ep} \), respectively. It is desirable that the structure have some measure of stiffness so that it can perform its structural application. Strain energy is chosen as an objective to capture the stiffness. It is also necessary that a measure of the sensing signal be maximized. This is acheived via maximization of Resistance change in the presence of strain [22, 23]. These objectives will be shown to be competing for a limited amount of CNT, with the stiffness optimization wanting to
place material in locations that may be disadvantageous for sensing, and vice versa. The problem is solved using an epsilon-constraint optimization, in which the strain energy constraint, objective function decrease, and optimality tolerances are used unless otherwise specified. This problem is solved using SQP optimization within Matlab’s fmincon optimization suite [27]. Default constraint, objective function decrease, and optimality tolerances are used unless otherwise specified.

3. Analysis and sensitivity formulation

3.1. Micromechanics

Micromechanics laws relate the design variables to local Young’s Modulus, resistivity, and piezoresistive constant in a given element. It is assumed that within an element the CNT are well dispersed and randomly oriented, giving effectively isotropic properties.

3.1.1. Young’s modulus. At low volume fractions the effective Young’s modulus of a CNT-epoxy composite linearly increases as more CNT are added [28]. A rule of mixtures model is used to approximate the composite effective Young’s modulus. The rule of mixtures equation is:

\[ E_v = E_{CNT} v_e + E_{mat} (1 - v_e), \]  

where \( E_v \) represents the local effective Young’s Modulus of the \( e \)th element, and \( v_e \), the local volume fraction of CNT in the \( e \)th element. \( E_{CNT} \) is the modulus of the CNTs, and \( E_{mat} \) is the modulus of the matrix. By nature of being the highest possible bound on effective modulus, the rule of mixtures model for stiffness acts to add conservatism to the sensing objective, which will be shown to be dependent on strain. The sensitivity of the Young’s modulus with respect to a change in the volume fraction is

\[ \frac{dE_v}{dv_e} = E_{CNT} - E_{mat}. \]  

3.1.2. Electrical resistivity. Small increases in CNT volume fraction can drastically decrease effective resistivity [7]. This behavior is seen to be nonlinear even at low volume fractions, requiring use of an inverse rule of mixtures model [19]. Effective resistivity is isotropic and given as

\[ \rho_{0e} = \frac{1}{\frac{\rho_{0e}^{CNT}}{v_e} + \frac{1 - v_e}{\rho_{0e}^{mat}}}, \]  

where \( \rho_{0e} \) is the effective resistivity of the \( e \)th element with a local CNT volume fraction \( v_e \). The CNT and matrix resistivities are given by \( \rho_{0e}^{CNT} \) and \( \rho_{0e}^{mat} \), respectively. The sensitivity is given by

\[ \frac{d\rho_{0e}}{dv_e} = \frac{1}{\rho_{0e}} - \frac{1}{(\rho_{0e})^2} \]  

3.1.3. Piezoresistive Constant. Piezoresistivity is a property that dictates how changes in strain influence resistivity. A piezoresistive constant, sometimes called a normalized gage factor, can be used to measure this property. The piezoresistive constant is denoted as the variable \( g_e \), and the local effective piezoresistive constant of the \( e \)th element is \( g_e \). Depending on the percolation threshold of a given CNT-Epoxy composite, the piezoresistive behavior can exhibit an almost discrete on/off behavior [29]. Below the percolation threshold the piezoresistivity is small, and at the percolation threshold the piezoresistivity is maximized. Continuing to add CNT beyond percolation CNT will reduce the piezoresistive constant [23, 30]. The percolation threshold of CNT-Epoxy composites can be as low as 0.0025% CNT volume fraction [31] but it is most common that this threshold is between 1.5% and 4.5% [29, 32], depending on type and processing method of the CNT. 2% volume fraction was
chosen for the percolation threshold. The effective piezoresistive constant is small below 2%, peaks at percolation, and decreases for larger volume fractions. A curve fit model is used to approximate this behavior, and is modeled after figure 8 in [33].

\[
\sigma = \frac{\sum_{i=1}^{3} A_i \tan((2i-1)\pi \nu_c) \nu_c \leq 0.15}{2(\cos(B_1 \pi \nu_c) + B_3)} \quad 0.015 < \nu_c \leq 0.02. \tag{7}
\]

The sensitivity of the piezoresistive constant to the CNT volume fraction is

\[
\frac{d\sigma}{d\nu_c} = \left\{ \begin{array}{l}
\sum_{i=1}^{3} A_i (2i - 1) \tan((2i - 1)\pi \nu_c) \frac{\partial}{\partial \nu_c} \left( \frac{\partial \nu_c}{\partial \nu_c} \right) \\
-2B_1 \pi \sin(B_1 \pi \nu_c) \\
-2C_1 \nu_c + C_2 \\
\end{array} \right. \quad 0.015 < \nu_c \leq 0.02 \quad 0.02 < \nu_c \leq 0.1 \tag{8}
\]

In equations (7) and (8), the constants \( A_1-A_3, B_1-B_2, \) and \( C_1-C_3 \) are selected to ensure that the curve is continuous and has a continuous first derivative. These parameters may be altered to tune the piezoresistive model to fit a specific manufacturing process and/or available experimental data. Table 1 shows the values identified for these constants in this paper.

### 3.1.4. Material properties

Material properties for CNT and Epon 862 are presented in Table 2 [32, 34]. It should be noted that the Poisson’s ratio of the nanocomposite is assumed to be a constant \( \nu = 0.3 \). Effective Poisson’s ratios of CNT-Epon composites were modeled using a Mori-Tanaka method in [35, 36], where it was found that for aligned CNT the composite effective properties were \( \nu_{12} = 0.377, \quad \nu_{23} = \nu_{13} = 0.263 \). For randomly oriented nanotubes it can be assumed that these values may be averaged, resulting in an effective Poisson’s ratio of 0.3.

The micromechanics equations are plotted against CNT volume fraction in figure 2.

### 3.2. Strain energy

The structure’s strain energy under prescribed loading is chosen as a measure of stiffness. A finite element model using 4 node bi-linear quadrilateral elements is used to solve both the mechanical and the electrostatic problems. For the mechanics, from which strain energy is calculated, each node has two degrees of freedom, \( u_x \) and \( u_y \). The element equilibrium equation for the 2D mechanics is

\[
K_e(\nu_c)u_e = f_e, \tag{9}
\]

where \( K_e \) is the element stiffness matrix, \( \nu_c \) the element CNT volume fraction, \( u_e \) the element displacement vector, and \( f_e \) the element load vector. The CNT volume fractions affect the strain matrix by modifying the constitutive matrix, \( D_e \).

\[
D_e(\nu_c) = E_e(\nu_c) \begin{bmatrix} E_{mod} & \nu E_{mod} & 0 \\ \nu E_{mod} & E_{mod} & 0 \\ 0 & 0 & G_{mod} \end{bmatrix}, \tag{10}
\]

where \( E_{mod} = \frac{1}{1-\nu^2} \) and \( G_{mod} = \frac{1}{2(1+\nu)} \). The element stiffness matrix can be written as

\[
K_e = \int_{\varepsilon} \int_{\eta} B_i^T D_e B_i |J| d\varepsilon d\eta, \tag{11}
\]

where \( B_i \) is the mechanical strain-displacement matrix and \( |J| \) is the determinant of the element Jacobian matrix. \( K_e \) is computed for each element and assembled into a global stiffness matrix, \( K \). The symmetry boundary conditions specify which \( u_x \) and \( u_y \) are set to 0, and the problem is solved for the remaining displacements. The strain energy is then computed as

\[
U = \frac{1}{2} u^T K u. \tag{12}
\]

The sensitivity of stiffness-based topology optimization problems is well studied, and the sensitivity of the strain energy is shown via a self-adjoint solution [15, 16] to be

\[
\frac{\partial U}{\partial \nu_c} = -\frac{1}{2} u^T \frac{\partial K_e}{\partial \nu_c} u_c, \tag{13}
\]

where the sensitivity of the stiffness matrix is dependent only on the sensitivity of the constitutive matrix.

\[
\frac{\partial K_e}{\partial \nu_c} = \int_{\varepsilon} \int_{\eta} B_i^T \frac{\partial D_e}{\partial \nu_c} B_i |J| d\varepsilon d\eta \tag{14}
\]

and as the element Young’s modulus has been factored out of \( D_e \) the sensitivity may be easily computed.

\[
\frac{\partial D_e}{\partial \nu_c} = \frac{\partial E_e}{\partial \nu_c} \begin{bmatrix} E_{mod} & \nu E_{mod} & 0 \\ \nu E_{mod} & E_{mod} & 0 \\ 0 & 0 & G_{mod} \end{bmatrix}. \tag{15}
\]

### 3.3. Resistance change due to strain

Gage factor is defined as the change in resistance between the strain and unstrained cross section divided by the unstrained resistance and the strain, and is a standard measure of sensing. Maximizing the resistance change between the strained and unstrained structure leads to an increase in signal-to-noise ratio in strain sensing.
3.3.1. Electric current. The electrostatics continuity equation states that the divergence of the current density ($\Psi$) is 0.

$$\nabla \cdot \Psi = 0. \quad (16)$$

Current density is related to electric conductivity ($\sigma$) and the electric field ($E$) via Ohm’s law as

$$\Psi = \sigma E. \quad (17)$$

The electric field is the negative of the gradient of the potential. Substituting this into equation (16) gives

$$\nabla \cdot \Psi = -\nabla \cdot (\sigma \nabla \phi) = 0. \quad (18)$$

In the 2D case the electric potential varies in the $z$ and the $y$ directions, $\phi = \phi(z, y)$. Conductivity may also change in both directions, $\sigma = \sigma(z, y)$. Rewriting the equation gives

$$\frac{\partial}{\partial z} \left( \sigma(z, y) \frac{\partial \phi(z, y)}{\partial z} \right) + \frac{\partial}{\partial y} \left( \sigma(z, y) \frac{\partial \phi(z, y)}{\partial y} \right) = 0. \quad (19)$$

The governing equations are discretized via the finite element method, resulting in the algebraic equations

$$C \phi = f \quad (20)$$

or, for a given element

$$C_e \phi_e = f_e \quad (21)$$

where $C_e$ is the element electrostatic ‘stiffness’ matrix, $\phi_e$ is the element electric potential vector, and $f_e$ is the element current vector. The electrostatic version of the stiffness matrix depends on the conductivity matrix $\sigma$.

$$C_e(\sigma) = \int_{\xi} \int_{\eta} B^T \sigma B |J| d\xi d\eta, \quad (22)$$

where $B$ is the gradient matrix, $|J|$ is the determinant of the element Jacobian, and $\sigma$ is the element conductivity, which will vary between the strained and unstrained problems.

Equation (20) is divided into submatrices based on which degrees of freedom are constrained. The subscript $u$ denotes degrees of freedom which are unspecified, but on the boundary. The subscript $s$ indicates these degrees of freedom are part of the boundary condition, and have their electric potential specified. This represents specifying the placement of electrodes on the structure. Finally, the subscript $ed$ indicates degrees of freedom on the interior of the structure.

$$\begin{bmatrix} C_{uu} & C_{us} & \phi_u \\ C_{us}^T & C_{ss} & \phi_s \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \phi_u \\ \phi_s \\ \phi_{ed} \end{bmatrix} = \begin{bmatrix} f_u \\ f_s \\ 0 \end{bmatrix}. \quad (23)$$

or, in simplified form: $\hat{C} \phi = b$. Here the symbol $I$ is used to represent the identity matrix.

Total current, $I_{bc}$, is measured as the summation of the nodal currents across a boundary electrode. The vector $q$ is created to aid in the summation. $q$ has a value of 1 for degrees of freedom on the boundary electrode to be summed over, and is 0 for the degrees of freedom on the other boundary electrode.

$$I_{bc} = q^T \begin{bmatrix} C_{uu} & C_{us} & C_{ss} \end{bmatrix} \phi = p^T \phi. \quad (25)$$

For the unstrained calculation an uncoupled adjoint method is used to obtain the sensitivity of the current. For this is is convenient to rearrange equation (24).

$$\begin{bmatrix} C_{uu} & 0 \\ C_{us}^T & 0 \\ C_{ss} \end{bmatrix} \begin{bmatrix} \phi_u \\ \phi_s \end{bmatrix} = \begin{bmatrix} -C_{uu} \phi_{ed} \\ -C_{us} \phi_{ed} \end{bmatrix} \quad (26)$$

or $\tilde{C}y = b$. The current is then given as

$$I_{bc} = \begin{bmatrix} 0 & 0 & q \end{bmatrix}^T y. \quad (27)$$
The adjoint equation is then formed
\[
C^T \dot{\lambda} = \frac{\partial I_{bc}}{\partial y} = q^T
\]  
(28)
which is solved for \(\dot{\lambda}\). Finally, the sensitivity equation is
\[
\frac{dI_{bc}}{dV_e} = \frac{\partial I_{bc}}{\partial y} + \lambda^T \left( \frac{dF}{dy} - dC \frac{d\phi}{dV_e} \right)
\]
(29)
Here the form of \(I_{bc}\) is convenient in that \(\frac{dI_{bc}}{dV_e} = 0\).

Furthermore, it is noted that \(\frac{dI_{bc}}{dV_e}\) may be rearranged, as it is a derivative of the original electrostatic equations, \(C\phi = f\)
\[
\frac{d}{dV_e} \begin{bmatrix} -C_{uu} \phi_{0u} \\ -C_{uv} \phi_{0v} \\ -C_{uu} \phi_{0u} \end{bmatrix} - \frac{d}{dV_e} \begin{bmatrix} C_{uu} & C_{uv} & 0 \\ C_{uv} & C_{vv} & 0 \\ C_{uu} & C_{uv} & -I \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = -dC \frac{d\phi}{dV_e}
\]
resulting in the final set of sensitivity equations
\[
\frac{dI_{bc}}{dV_e} = -\lambda^T dC \frac{d\phi}{dV_e} = -\lambda \left( B^T \frac{\partial \sigma}{\partial y} B \right) I_e.
\]
(31)

For the case of the unstrained resistance
\[
\frac{\partial \sigma}{\partial y_e} = \frac{\partial}{\partial V_e} \begin{bmatrix} 1/\rho_0 & 0 \\ 0 & 1/\rho_0 \end{bmatrix},
\]
(32)
where the sensitivities of the resistivity are provided by the micromechanics equations.

Adding the piezoresistive term alters the conductivity matrix, as a piezoresistive term is added to the resistivity as
\[
\begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_6 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} + \begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{12} & g_{11} & 0 \\ 0 & 0 & g_{66} \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \gamma_6 \end{bmatrix} \rho_0
\]
(33)
there are potentially three different resistivities, related to the three strain components via the \(g\) matrix. \(\rho_0\) is the unstrained resistivity, \(\epsilon\) is the strain vector, and \(g\) is the piezoresistive constant matrix. The resistivity values are used to assemble the element conductivity matrix. Here both \(\rho_0\) and \(g\) are explicit functions of the CNT volume fraction in a given element, \(V_e\). This formulation follows \[1\] and \[2\] and assumes that the through-thickness strains i.e. \(\epsilon_3\), \(\gamma_4\), and \(\gamma_5\) are not significant.

The element conductivity matrix for the strained problem is given as \(\tilde{\sigma}\) and is obtained via inversion of the resistivity matrix.
\[
\tilde{\rho} = \begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_6 \end{bmatrix}
\]
(34)
\[\tilde{\sigma} = \tilde{\rho}^{-1}.
\]
(35)

The sensitivities of the conductivity matrix with respect to volume fraction must be obtained to calculate the sensitivity of the resistance change objective. These sensitivities are
\[
\frac{\partial \tilde{\sigma}}{\partial V_e} = -\tilde{\rho}^{-1} \frac{\partial \tilde{\rho}}{\partial V_e} \tilde{\rho}^{-1}
\]
and
\[
\frac{\partial \rho_1}{\partial V_e} = \rho_0' (1 + g_{11} \epsilon_1 + g_{12} \epsilon_2) + \rho_0 (g_{11}' \epsilon_1 + g_{12}' \epsilon_2)
\]
(37)
\[
\frac{\partial \rho_2}{\partial V_e} = \rho_0' (1 + g_{12} \epsilon_1 + g_{11} \epsilon_2) + \rho_0 (g_{12}' \epsilon_1 + g_{11}' \epsilon_2)
\]
(38)
and
\[
\frac{\partial \rho_6}{\partial V_e} = \rho_0 (g_{66}' \gamma_6).
\]
(39)

\(g_{1i}'\) and \(\rho_0'\) indicate derivatives of the micromechanics equations with respect to the local volume fraction. In literature \[7, 35\] the shear terms of the CNT-polymer composite piezoresistivity were seen to be small, and thus for the representative model used herein it is assumed that \(g_{11} = g_{12} = g\) and \(g_{66} = 0\), where \(g\) is provided via equation \(7\).

General forms of coupled adjoint sensitivities are adapted for the sensitivity of the coupled piezoresistive problem \[37\]. The equilibrium equations are labeled \(R = Ku - f\) and \(R = C\phi - I\). The objective functions are \(F_1 = U\) for strain energy and \(F_2 = I_{bc}\) for the strained current out of the boundary electrode. The strained current is considered here as it is the term in the resistance change that includes the coupling. In matrix form
\[
R = \begin{bmatrix} R_1(v, u) \\ R_2(v, u, \phi) \end{bmatrix}
\]
(40)
\[
F = \begin{bmatrix} F_1(v, u) \\ F_2(v, u, \phi) \end{bmatrix}
\]
(41)

The total derivative is given as
\[
\frac{dF}{dy_e} = \frac{\partial F}{\partial y_e} + \frac{\partial F}{\partial y_e} \frac{\partial y_e}{\partial y_e},
\]
(42)
where \(y\) is the state variable vector \(y = [u, \phi]\). The derivatives of the equilibrium equations are
\[
\frac{dR}{dy_e} = \frac{\partial R}{\partial y_e} + \frac{\partial R}{\partial y_e} \frac{\partial y_e}{\partial y_e} = 0
\]
(43)
which can be solved for \(\frac{\partial y_e}{\partial y_e}\). The total derivative is reformulated to include the sensitivity of the residuals multiplied by the adjoint variable \(\lambda\).
\[
\frac{dF}{dy_e} = \frac{\partial F}{\partial y_e} - \lambda^T \frac{\partial R}{\partial y_e},
\]
(44)
where \(\lambda\) is obtained through the solution of the adjoint equation in equation \(45\)
\[
-\frac{\partial R^T}{\partial y} \lambda = \frac{\partial F^T}{\partial y}.
\]
(45)
For the mechanical and electrostatic coupled problem this equation expands to
\[
- \begin{bmatrix} R_{1,\phi}^T & R_{2,\phi}^T \\ R_{1,\phi}^T & R_{2,\phi}^T \end{bmatrix} \begin{bmatrix} \lambda_{\mu u} & \lambda_{\phi u} \\ \lambda_{\mu \phi} & \lambda_{\phi \phi} \end{bmatrix} = \begin{bmatrix} F_{1,u} \\ F_{1,\phi} \end{bmatrix},
\]

where the subscript, \( u \) and, \( \phi \) indicate derivatives of the residuals and objectives with respect to that state variable. If only the strained current sensitivity is required (as the strain energy sensitivity has been solved via self-adjoint), this reduces to
\[
- \begin{bmatrix} R_{1,\phi}^T & R_{2,\phi}^T \\ R_{1,\phi}^T & R_{2,\phi}^T \end{bmatrix} \begin{bmatrix} \lambda_{\mu u} \\ \lambda_{\phi u} \end{bmatrix} = \begin{bmatrix} F_{2,u} \\ F_{2,\phi} \end{bmatrix}.
\]

Similarly, partitioning equation (44) to only consider the strained current objective results in an updated version of equation (31).
\[
\frac{dF_{2}}{dV_{c}} = - \lambda_{\mu u}^T \frac{\partial K}{\partial V_{c}} - \lambda_{\phi u}^T \frac{\partial C}{\partial V_{c}} \phi.
\]

The adjoint variables and the sensitivities of the stiffness and conductivity matrices to volume fraction changes must now be obtained. The sensitivities of the residuals with respect to the states are
\[
\begin{align*}
R_{1,u} &= \frac{\partial(Ku - f)}{\partial u} = K \\
R_{2,u} &= \frac{\partial(C\phi - f)}{\partial u} = \frac{\partial C}{\partial \phi} \\
R_{1,\phi} &= 0 \\
R_{2,\phi} &= \frac{\partial(C\phi - f)}{\partial \phi} = C.
\end{align*}
\]

The sensitivities of the objectives with respect to the states are
\[
\begin{bmatrix} F_{2,u} \\ F_{2,\phi} \end{bmatrix} = \begin{bmatrix} \frac{\partial H_{bc}}{\partial u} \\ \frac{\partial H_{bc}}{\partial \phi} \end{bmatrix}
\]

\[
\frac{\partial H_{bc}}{\partial u} = \frac{\partial p^T \phi}{\partial u}
\]

\[
\frac{\partial H_{bc}}{\partial \phi} = p^T
\]

and the adjoint equation is reposed as
\[
- \begin{bmatrix} K^T & 0^T \\ \phi^T & C^T \end{bmatrix} \begin{bmatrix} \lambda_{\mu u} \\ \lambda_{\phi u} \end{bmatrix} = \begin{bmatrix} \partial q^T \phi \\ q^T \end{bmatrix}.
\]

As \( p = q^T C \), and \( q \) is just a selection vector of 1’s and 0’s, the only remaining term to solve is \( R_{2,u} \) in equation (50).

This may be computed on an element-wise basis and then assembled into a global sensitivity matrix, similar to the finite element assembly of the stiffness and conductivity matrices. For an element \( e \)
\[
\frac{\partial R_{e}}{\partial u_e} = B_{e} J_{e} D_{e},
\]

where
\[
B_{e} = -B_{e}^T \phi_e
\]

and
\[
J_{e} = \begin{bmatrix} j_{ie} & 0 \\ 0 & j_{ie} \end{bmatrix}
\]

where the the \( j_{ie} \) vector has 2 components, via
\[
J_{e} = \hat{z} B_{e} \phi_e |J_e|.
\]

and
\[
D_{e} = \rho_{0e} \hat{g}_e B_{e}
\]

here \( \rho_{0e} \) is the local unstrained resistivity, \( \hat{g}_e \) is the local piezoresistive matrix, \( B_{e} \) is the element strain-displacement matrix, \( B_{e} \) is the element electrostatic-gradient matrix (the electrostatic analog to the strain-displacement matrix), \( \hat{z}_e \) is the element conductivity matrix, and \( |J_e| \) is the determinant of the element Jacobian.

3.3.2. Resistance change. Resistance change due to strain, \( \frac{\Delta R}{R_0} \), is measured as the difference in resistance between the unstrained structure (\( R_0 \)) and the resistance of the strained structure (\( R_e \)), normalized by the unstrained resistance i.e.
\[
\frac{\Delta R}{R_0} = \frac{R_e - R_0}{R_0}.
\]

Resistance is related to current through Ohm’s law, \( R = \frac{V}{I} = \frac{\Delta \phi}{I_{bc}} \). \( \Delta \phi \) is the prescribed potential difference across the electrodes, and is a constant for both the strained and unstrained resistances. This allows for simplification of the resistance change function.
\[
\frac{\Delta R}{R_0} = \frac{I_{bc} - I_{bc}}{I_{bc}} = \frac{I_{bc}}{I_{bc}} - 1.
\]

The sensitivity is then
\[
\frac{\Delta R'}{R_0} = \frac{I_{bc} - I'_{bc}}{I_{bc}} = \frac{I'_{bc}}{I_{bc}}.
\]

4. Optimal topologies with a fixed electrode

The coupled optimization is performed using the epsilon-constraint method introduced in equation (2). Single objective optimization with a uniform CNT distribution is used to obtain utopia points that inform the bounds on the strain energy epsilon-constraint. Global volume fractions of 2% and
5% are considered, as well as a case without a global volume fraction constraint.

Pareto fronts for the plate with a hole are plotted in figure 3. The top left subplot compares Pareto fronts across all three volume fraction constraint cases, and the remaining plots isolate a single constraint case.

The vertical axis in figure 3 marks the stiffness performance and the horizontal axis marks the sensing performance, with higher values of both being preferred. Figure 4 plots the optimal stiffness and sensing values against the volume fraction constraint. Note that because the side constraints on each element restrict the local volume fraction to be less than or equal to 10%, the unconstrained case can have a maximum global volume fraction of 10%.

The optimal stiffness is dominated by the volume fraction constraint, with the unconstrained case being 40% more stiff than the 5% constrained case, which was itself twice as stiff as the 2% constrained case. The topologies that perform the best in stiffness are plotted for each constraint level in figure 5 alongside their volumetric strain fields.

As adding more CNT will always increase the local Young’s modulus, the unconstrained optimum for stiffness...
maximization is a topology with maximum CNT in each element. Once the volume fraction constraint is activated and begins to restrict CNT usage, the stiffness is maximized by placing higher volume fractions of CNT near the right edge of the hole, minimizing the stress concentration. Another common feature in both the 2% and 5% topologies is a stiffening arc leading up and around the net-negative strain region. Away from the hole the strains are relatively uniform, and the optimizer has little preference as to volume fraction or specific topology in this region.

When comparing sensing performance the 5% constrained and unconstrained design both dominate the 2% constrained designs, but there is little to no increase in the sensing objective when relaxing the constraint beyond 5%. The optimal sensing topologies for each constraint level are plotted in figure 6 alongside their local resistivity changes due to strain.

Sensing is optimized by placing highly piezoresistive-near 2% CNT volume fraction-material near the highly strained right edge of the hole. A conductive path connecting this area to the electrode on the right vertical edge is also common across all of the designs. A region of low CNT volume fraction material in the center of the design, common across all three constraint levels, seems to be a preferred feature of the topology. The optimizer is manipulating the strain field to concentrate the load in the highly piezoresistive region, resulting in a higher sensing performance. Of course, carving out a large piece of the design and dumping more load into a relatively compliant section of the structure may not make for a good structure, but it makes for the best sensor.

Figure 7 characterizes the transition from optimal structure to optimal sensor. This figure shows four of the Pareto Optimal topologies from the 5% constraint case along with their respective stiffness and sensing performance. As the stiffness epsilon-constraint is relaxed, the region of low CNT in the center of the design grows, trading stiffness for improved sensing.

5. A surrogate model for the designed electrode

In order to obtain measurable resistance change due to strain there must be a path of conductive CNT linking the electrodes. The location of the electrodes dictates where this path must form, and so it is of interest to allow the optimizer to tailor the electrode in addition to the CNT distribution. It has been seen that this can serve to both increase sensing performance and partially decouple stiffness and sensing objectives [14]. This presents unique challenges in that the prescribed electrodes exist as discrete degrees of freedom in a finite element mesh. Including the electrode placement within the optimization necessitates either the use of a mixed-variable optimizer or a way of converting the discrete electrode variables into pseudo-continuous variables.

Surrogate models, covered in depth in [38], use curve fitting and statistics to interpolate the behavior of a function between discrete evaluation points. Unless remeshing is
performed at every optimization iteration, the boundary nodes on a mesh are fixed points and the optimal location of an electrode may well lie between nodes on the mesh. A surrogate model allows for interpolation of the resistance change performance for electrodes that end between nodes. A quadratic response surface model is developed for this purpose.

5.1. The quadratic surrogate model

The design variable vector is updated as $x = [v, b]$, where $x$ are the continuous design variables. $v$ is comprised of the CNT volume fractions, $v$, and the continuous electrode index variables, $b$. Here the problem is simplified such that only a single electrode is designed, i.e. $b = [b_1; b_2]$ where $b_1$ and $b_2$ mark the starting and ending location of the variable electrode. The electrode along the circular edge was chosen as the variable electrode, as this area has been seen to be important in the results presented in the previous section. All nodes on the specified edge that fall between $b_1$ and $b_2$ are considered part of the electrode. The performance and sensitivity of the surrogate model is formulated as follows.

First, the continuous electrode variables are rounded to the nearest discrete value, $b = \text{round}(b)$. The remainder, $r = b - \text{round}(b)$, will also be used. As $b$ is discrete, it is used within the established analysis and sensitivity to compute the resistance change at the rounded electrode location.

The resistance change objective at the rounded electrode values is

$$f_n = \frac{\Delta R}{R_0} (v, b)$$

and the sensitivity of the objective at the rounded values with respect to changes in the volume fractions is

$$\frac{df_n}{dv} = \frac{d}{dv} \frac{\Delta R}{R_0} (v, \bar{b}).$$

To use a quadratic surrogate approximation the function needs to be evaluated at different points of $b$. The $\delta$ matrix is created as

$$\delta = \begin{bmatrix} 1 & -1 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & -1 & 1 & -1 \end{bmatrix}$$

and the discrete electrode objective function is evaluated for each column of $\delta$.

$$f_{\delta_i} = f (v, \bar{b} + \delta_i).$$

These function evaluations are used to form the coefficients for the quadratic equation that may take the form

$$F = f_n + B^T r + \frac{1}{2} r^T C r.$$

Coefficients for the $B$ vector and $C$ matrix come from finite difference approximations. $B$ is comprised of the first order finite difference coefficients:

$$B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} = \begin{bmatrix} (f_{\delta_1} - f_{\delta_2})/2 \\ (f_{\delta_3} - f_{\delta_4})/2 \end{bmatrix}.$$
matrix of the second order finite difference coefficients:

\[
C = \begin{bmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{bmatrix}
\]

(71)

\[
C_{11} = \frac{\partial^2 f}{\partial b_1^2} \approx f_{b_1} - 2f_a + f_{b_2}
\]

(72)

\[
C_{22} = \frac{\partial^2 f}{\partial b_2^2} \approx f_{b_2} - 2f_a + f_{b_1}
\]

(73)

\[
C_{12} = \frac{\partial^2 f}{\partial b_1 \partial b_2} \approx \frac{f_{b_1} - f_{b_2} - f_{b_3} + 2f_a - f_{b_1} + f_{b_2} + f_{b_3}}{2}.
\]

(74)

The sensitivity of the surrogate model to changes in the electrode variables is then

\[
\frac{\partial F}{\partial b_i} = B_i + C_{ij} r_j
\]

(75)

and the sensitivity with respect to all design variables:

\[
\frac{dF}{dx} = \left[ \frac{\partial F}{\partial b_1}, \frac{\partial F}{\partial b_2} \right] \frac{dr}{dx}
\]

is obtained from equation (66).

A detailed verification and validation of the surrogate model can be found in [14].

6. Results for simultaneous optimization of topology and boundary electrode

The Pareto Fronts for designed electrodes and topology are plotted alongside the optima with only the designed topology in Figure 8. The ‘x’ indicates an optima obtained with the designed electrode, the ‘o’ is reprinted from the fixed electrode results in section 4.

As the stiffness objective is independent of electrode placement, the stiffness-optimal designs show little to no improvement between fixed and designed electrode cases. As the strain energy epsilon-constraint is relaxed the design that includes the variable electrode dominates its fixed electrode counterpart. Table 3 compares sensing performance for select fixed and variable electrode designs. Each comparative case shows the sensing performance for a matching stiffness performance. Optimizing the electrode offers a significant sensing across all constraint levels, at least a 1.46 times increase in sensing for the values shown. This increase is more significant, at least a 1.81 times increase for 5% and a 1.88 times increase for the unconstrained case, as the volume fraction constraint is relaxed.

Figure 9 plots two topologies with the same stiffness for a constraint volume fraction of 5%. The first is optimized with
Figure 8. 2D plane stress Pareto Fronts comparing optima with designed electrode and topology to optima with just designed topology.

Figure 9. Left: Optimized topology with a 0.214 stiffness requirement and fixed electrode. Right: Optimized topology with a 0.214 stiffness requirement and an optimized electrode.

Table 3. Comparing sensing performance for fixed and designed electrode.

|                  | 2% Fixed electrode | 2% Optimized electrode | Ratio | 5% Fixed electrode | 5% Optimized electrode | Ratio | Unconstrained Fixed electrode | Unconstrained Optimized electrode | Ratio |
|------------------|--------------------|------------------------|-------|--------------------|------------------------|-------|-------------------------------|-----------------------------------|-------|
|                  | 0.0104             | 0.0151                 | 1.46  | 0.0113             | 0.0204                 | 1.81  | 0.0093                        | 0.0177                           | 1.89  |
|                  | 0.0120             | 0.0193                 | 1.62  | 0.0144             | 0.0274                 | 1.90  | 0.0146                        | 0.0274                           | 1.88  |
a fixed electrode, and the second is optimized with a variable inner electrode. The purple bar indicates the electrode location along the inner edge for both designs.

The topology with the designed electrode places stiff material (red elements) around the edge of the hole, next to the piezoresistive material. This is a feature not shared by the topology with the fixed electrode, and allows for a larger cutout in the center-right of the design while still satisfying the strain energy epsilon-constraint. Red elements are both stiff and conductive, and as such red elements attached to the inner electrode form a path of least resistance that would bypass the sensing elements in the bottom right of the hole section. With a full length electrode, there is no way to bring this stiff material down to the circular edge without sacrificing sensing performance. Another advantage of the designed electrode is that it is concentrated only at the region of highest sensing. This electrode design is consistent across the best sensing topologies for all volume fraction constraints, which are shown in figure 10.
In all cases, once the stiffness requirement is sufficiently reduced the designed electrode optima dominate the fixed electrode optima. This stiffness threshold corresponds to when the optimizer no longer needs stiff, poor sensing material to occupy the location of the stress concentration around the hole. For designs with intermediate stiffness requirements shifting the electrode allows for unique topologies that satisfy stiffness without subverting the sensing-optimal conductive path. Even when the stiffness constraint is completely relaxed the optimized electrode works with the topology to force the current to flow through the best sensing regions of the design. The development of the topology with a fixed electrode, and then a surrogate model was used to incorporate the electrode into the design. Main results of this work are presented as:

1. Stiffness is maximized by placing high volume % CNT elements around the stress concentrations.
2. Sensing is maximized by placing highly piezoresistive elements around the stress concentrations, forming conductive paths between electrodes, and manipulating the load path to concentrate loads in the best sensing region.
3. Stiffness monotonically increases with available CNT, sensing is less depending on material available after a threshold, around 5% for the cases presented here.
4. Adding the electrode to the optimization allows for tailored conductive paths, increasing stiffness for all volume fraction cases once the stiffness requirement is low enough to allow location of piezoresistive material around the designed electrode.

7. Conclusions

This paper presented a method for optimal distribution of a limited amount of CNTs within an epoxy matrix to provide Pareto-Optimal designs for stiffness and strain sensing objectives. Analytic analysis and sensitivity equations based on micromechanics and FEA were developed and used within an SQP optimization routine. Designs were first optimized with a fixed electrode, and then a surrogate model was used to incorporate the electrode into the design. Main results of this work are presented as:

1. Stiffness is maximized by placing high volume % CNT elements around the stress concentrations.
2. Sensing is maximized by placing highly piezoresistive elements around the stress concentrations, forming conductive paths between electrodes, and manipulating the load path to concentrate loads in the best sensing region.
3. Stiffness monotonically increases with available CNT, sensing is less depending on material available after a threshold, around 5% for the cases presented here.
4. Adding the electrode to the optimization allows for tailored conductive paths, increasing stiffness for all volume fraction cases once the stiffness requirement is low enough to allow location of piezoresistive material around the designed electrode.

ORCID iDs

Ryan Seifert @ https://orcid.org/0000-0002-4612-0011
Gary Seidel @ https://orcid.org/0000-0002-1156-5010

References

[1] Sairajan K K, Aglietti G S and Mani K M 2016 Acta Astronaut. 120 30–42
[2] Roberts S C and Aglietti G S 2008 Proc. IMechE 222 41–51
[3] Giurgiutiu V, Zagrai A and Bao J J 2002 Struct. Health Monit. 1 41–61
[4] Taleja R and Singh C V 2012 Damage and Failure of Composite Materials 1st edn (Cambridge, NY: Cambridge University Press) (https://doi.org/10.1017/CBO9781139016003)
[5] Obitayo W and Liu T 2012 J. Sens. 2012 1–15
[6] Gang Yin N H 2011 J. Compos. Mater. 45 1315–23
[7] Chaurasia A K and Seidel G D 2014 J. Intell. Mater. Syst. Struct. 25 2141–64
[8] Ivanova O, Williams C and Campbell T 2013 Rapid Prototyping J. 19 353–64
[9] Postiglione G, Natale G, Grifﬁni G, Levi M and Turri S 2015 Composites A 76 110–4
[10] Maute K, Tkachuk A, Wu J, Qi H J, Ding Z and Dunn M L 2015 J. Mech. Des. 137 111402
[11] Rubio W M, Silva E and Nishikawa S 2008 Struct. Multidiscip. Optim. 6 571–83
[12] Giusti S M, Mello L A M and Silva E C N 2014 Struct. Multidiscip. Optim. 50 453–64
[13] Mello L A M, Takezawa A and Silva E C N 2012 Smart Mater. Struct. 21 085029
[14] Seifert D R 2018 Topology optimization of multifunctional nanocomposite structures PhD Thesis Virginia Tech
[15] Bendsøe M P and Sigmund O 2004 Topology Optimization (Berlin: Springer) (https://doi.org/10.1007/978-3-662-05086-6)
[16] Deaton J D and Grandhi R V 2014 Struct. Multidiscip. Optim. 49 1–38
[17] Swan C C and Kosaka I 1997 Int. J. Numer. Methods Eng. 40 3033–57
[18] Voigt W 1889 Ann. Phys., Lpz. 274 573–87
[19] Reuss A 1929 ZAMM-J. Appl. Math. Mech./Z. Angew. Math. Mech. 9 49–58
[20] Eshelby J D 1957 Proc. R. Soc. A 241 376–96
[21] Mori T and Tanaka K 1973 Acta Metall. 21 571–4
[22] Oskouyi A, Sundararaj U and Mertiny P 2014 Materials 7 2501–21
[23] Hu N, Fukunaga H, Atobe S, Liu Y and Li J 2011 Piezoresistive strain sensors made from carbon nanotubes based polymer nanocomposites Sensors 11 10691–723
[24] Ehrlogg M and Gandibleux X 2000 OR-Spektrum 22 425–60
[25] Hwang C L and Masud A S M 1979 Methods for multiple objective decision making Multiple Objective Decision Making—Methods and Applications (Berlin: Springer) pp 21–83
[26] Mavrotas G 2009 Applied mathematics and computation 213 455–65
[27] fmincon https://mathworks.com/help/optim/ug/fmincon.html
[28] Seidel G D and Lagoudas D C 2006 Mech. Mater. 38 884–907 advances in Disordered Materials
[29] Bauhower W and Kovacs J Z 2009 Compos. Sci. Technol. 69 1486–98
[30] Keulemans G, Ceyssens F, De Vorder M, Seo J W and Puers R 2010 Fabrication and characterisation of carbon nanotube composites for strain sensor applications MM2010 21 pp 231–4
[31] Sandler J, Kirk J, Kinloch I, Shaffer M and Windle A 2003 Polymer 44 5893–9
[32] Schueler R, Petermann J, Schulte K and Wentzel H P 1997 J. Appl. Polym. Sci. 63 1741–6
[33] Ren X and Seidel G D 2013 Compos. Interfaces 20 693–720
[34] Zhu R, Pan E and Roy A 2007 Mater. Sci. Eng. A 447 51–7
[35] Chaurasia A K, Sengere E C, Talanadupula K K, Povolny S and Seidel G D 2014 J. Multifunctional Compos. 2 227–53
[36] Hammerand D C, Seidel G D and Lagoudas D C 2007 Mech. Adv. Mater. Struct. 14 277–94
[37] Martins J R R A and Huang J T 2013 AIAA J. 51 2582–99
[38] Swiler L P, Hough P D, Qian P, Xu X, Storlie C and Lee H 2014 Surrogate models for mixed discrete-continuous variables Constraint Programming and Decision Making (Berlin: Springer) pp 181–202