Genetic Algorithm for Material Optimization

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Introduction

The objective of this report is to analyze and optimize the design of a particle-doped composite. Given a set of desired material properties (such as mechanical, thermal, and electrical properties), we can develop an advanced material optimized for strength properties, electrical properties, and/or thermal properties by minimizing the concentration factors that limit the effectiveness of load sharing between different phases.[1] The applications of such an analysis is crucial to almost every engineering problem. Applications include developing a lighter, stronger airfoil, conductive phone charging cases, and super-conductors for telecommunications applications. A genetic algorithm is used to maximize the composite material properties. By combining materials in a particle-doped composite, an optimized composite can be developed.

Methodology

Effective Properties

Effective properties are micro-scale properties obeying the continuity assumptions between neighboring cells which compute the rough properties of a composite material. To analyze effective properties, the Hashin-Shtrikman (HS) boundaries are used. These boundaries are based on isotropy on infinite bodies assuming isotropic effective responses. Only the properties of the material and the volume fractions of the constituent materials are known. The HS bounds take a lower bound, $y^{*,-}$ and upper bound $y^{*,+}$, and compute the effective property of the mixture–a weighted average of the bounds [2]. The HS bounds for mechanical, thermal, and electrical properties relevant to this analysis are located in the Appendix along with descriptions of their significance.

$$y^{*,-} \leq y^{*} \leq Y^{*,+} \tag{1}$$

$$y^{*} = \gamma y^{*,-} + (1-\gamma) y^{*,+} \tag{2}$$

Concentration Factors and Load Sharing

While the effective properties are extremely useful to the performance of a material, it is not the sole predictor of performance. Consider a **phase one** rubber matrix used to produce conductive charging phone cases. Ideally, the phone case charges the phone wirelessly without large energy losses. A rubber matrix would be highly inefficient, as most of the charge is absorbed through the rubber matrix and released as heat. Doping the rubber with copper promotes the flow of electrons to the phone, in turn, improving charging efficiency. Using the previous example, the property we seek to minimize is joule-heating (the amount of heat generated from running a current through a material). One can determine the concentration factors of copper to satisfactorily minimize the heat generated by considering the **phase one** properties (rubber only) and **phase two** (rubber and copper). While the phone case is a single example, we seek to develop an optimization algorithm that considers several properties: mechanical, thermal, and electrical.

Mechanical load sharing will optimize the microstructure based on the stress and strain concentrations tensors used in previous projects [3]. For isotropic materials, the fraction of the total stress

carried by each phase can be determined by multiplying the concentration factors by their corresponding volume fractions. Electrical load sharing (discussed earlier) considers the phase-wise load shares of the Joule field, and finally, thermal load sharing for a two-phase mixture considers the concentration of the thermal fields in each phase.

Simulation for Material Optimization

Assumptions

The algorithm is applied to a base matrix with fixed material values using $\gamma = 0.5$. The design variables for the second phase matrix are defined as:

$$\Lambda = \kappa_2, \mu_2, \sigma_{e,2}, K_2, v_2 \tag{3}$$

where κ is the phase bulk modulus, μ_2 is the shear modulus, σ is the overall electrical conductivity, K is the effective thermal conductivity, and v is the volume fraction.

$$\begin{aligned}\Pi_{mechanical} = w_1|\frac{\kappa^{*,Des} - \kappa^*}{\kappa^{*,Des}}|^2 + w_1|\frac{\mu^{*,Des} - \mu^*}{\mu^{*,Des}}|^2 + \hat{w_3}|\frac{C_\kappa^{\sigma,2} - TOL_\kappa}{TOL_\kappa}|^2 \\ +\hat{w_4}|\frac{C_\mu^{\sigma,2} - TOL_\mu}{TOL_\mu}|^2 + \hat{w_5}|\frac{C_\kappa^{\sigma,1} - TOL_\kappa}{TOL_\kappa}|^2 + \hat{w_6}|\frac{C_\mu^{\sigma,1} - TOL_\mu}{TOL_\mu}|^2\end{aligned} \tag{4}$$

$$\Pi_{electrical} = w_1|\frac{\sigma_e^{*,Des} - \sigma_e^*}{\sigma_e^{*,Des}}|^2 + \hat{w_2}|\frac{C_{J1}C_{E1} - TOL_\sigma}{TOL_\sigma}|^2 + \hat{w_3}|\frac{C_{J2}C_{E1} - TOL_\sigma}{TOL_\sigma}|^2 \tag{5}$$

$$\Pi_{thermal} = w_1|\frac{K^{*,Des} - K^*}{K^{*,Des}}|^2 + \hat{w_2}|\frac{C_{q2} - TOL_K}{TOL_K}|^2 + \hat{w_3}|\frac{C_{q2} - TOL_K}{TOL_K}|^2 \tag{6}$$

With each property, thermal, mechanical, and electrical, we would like to combine all the variables into a single scalar value that can be minimized by the genetic algorithm. Objective cost functions for each material property are developed with weights (2,3,4), and the genetic algorithm combines the cost functions for each type of material property, optimizing all properties simultaneously with their associated weights.

$$\Pi_{Total} = W_1\Pi_{electrical} + W_2\Pi_{thermal} + W_3\Pi_{mechanical} \tag{7}$$

Results

The results from the genetic algorithm implementation using the combined cost function (5) are shown below. The implementation used 200 design strings per generation with ten children. Figure 1 shows the top 10 parent designs kept between each generation, indicating 180 total strings per generation. Each generation's best performing design follows a decreasing trend towards convergence, either following a plateau for several generations or decreasing. The algorithm rapidly localizes the desired parameters within the first five generations and slowly decays for the subsequent 4995 generations. The lowest costs for each design variable and the total costs are shown in Table 1.

Design	$\Lambda_\kappa * 10^{12}$	$\Lambda_\mu * 10^{12}$	Λ_K	$\Lambda_\sigma * 10^8$	Λ_v	Π
1	1.810	1.837	231.8	3.59	0.699	1.042
2	0.123	0.074	5.044	10.65	0.003	15.04
3	2.232	1.207	150.9	3.163	0.158	1.127
4	5.647	1.630	122.2	3.651	0.762	2.366

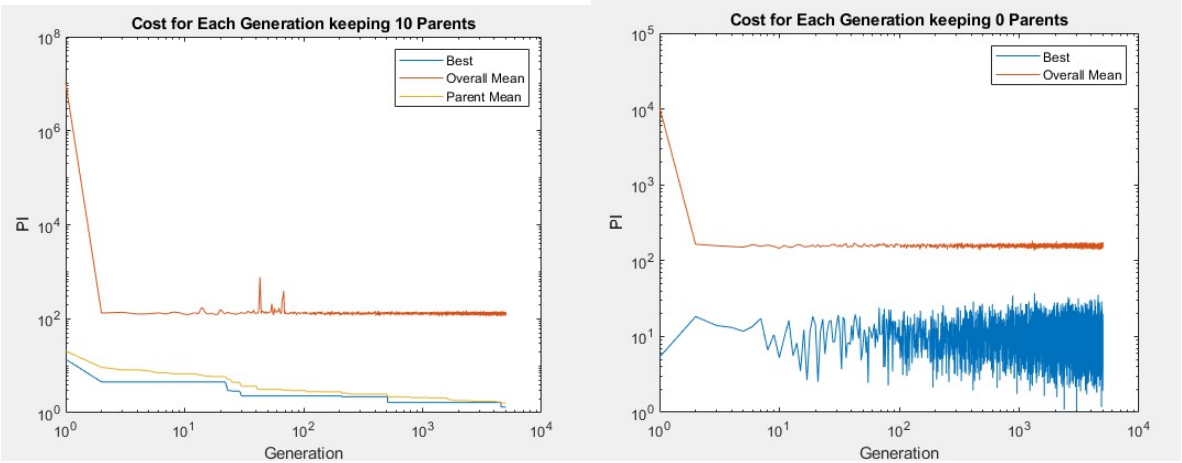
Table 1: Top 4 Designs for 10 Parents

The minimum total costs range from 15.04 to 1.042. This wide deviation in total costs can be compared by comparing the Λ_K values. Design 1 and Design 2 (lowest cost and highest cost) have $\Lambda_K = 231.8$ and $\Lambda_K = 5.044$ respectively. This contrast indicate a large dependence on the thermal conductivity

properties of the material. Cost can be minimized through high conductivity. Comparing between designs 2 and 3 is less visible, and there is no noticeable correlation that can be drawn from the total cost. Figure 2 shows the top 10 parents not being kept between each generation. Instead, only children and randomly generated design strings are used. For the second case, the top 10 parents were not retained between each generation. Only children and randomly generated strings are used. The top 10 performers quickly decreased in the first several generations, but the best performer did not follow this trend line. The best performers begin around 70, and slowly converge, sometimes increasing the cost, sometimes decreasing. When parents are not generated in the GA, there is no guarantee that the offspring will have a lower value, because the best parents were never conserved during the algorithm. The best performing designs are shown in Table 2.

Design	$\Lambda_\kappa * 10^{12}$	$\Lambda_\mu * 10^{12}$	Λ_K	$\Lambda_\sigma * 10^8$	Λ_v	Π
1	0.131	0.059	4.601	0.164	0.002	1.208
2	0.117	0.070	5.176	0.101	0.002	2.067
3	0.165	0.040	8.358	0.100	0.0032	1.267
4	0.120	0.048	8.340	0.1445	0.006	12.48

Table 2: Top 4 Designs for 0 Parents



Conclusion

Doped-composite materials have a range of properties which arrive from the constituent materials that can drastically affect the material characteristics. In this report, a simulation is developed to optimize the material properties of a doped composite by adjusting the thermal, mechanical, and electrical properties using convex combinations of the effective properties.

References

[1] Chien-hong Lin, Effective properties of 0–3, 1–3, and 2–2 composites based on unified unit-cell micromechanics model, Mechanics Research Communications, Volume 119, 2022,
[2] T. I. Zohdi, Modeling and Simulation Tools for Industrial Research Applications, Level 2 Course Notes, 2022
[3] Tristan Schwab, Deformation, https://calfdm.com/coursework