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Title:

Optimization of Micromechanical Densification Modeling Parameters for Copper Powder Using a Fuzzy Logic Based Multiobjective Genetic Algorithm

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Abstract

A fuzzy logic based multiobjective genetic algorithm (GA) was used to optimize the micromechanical densification modeling parameters such as that of Ashby's HIP 6.1 for copper powder. In addition to optimizing the 16 main parameters, the GA provides a quantitative measure of the sensitivity of the model to each parameter. While not a sensitivity analysis in the strictest sense, and highly stochastic in nature, this method is reliable and reproducible in optimizing parameters given any size data set and determining the impact on the model of slight variations in each parameter.

1.0 Introduction

1.1 Powder Processing

Dry powder pressing, be it uniaxial, isostatic, hot or cold has a number of technological advantages over other processing techniques. In addition to ease of fabrication, the use of powders helps to insure a random microstructure which usually results in isotropic thermo-mechanical properties of the final part. The three main advantages of dry pressing when making simple shapes, are speed, near net shaping, and minimal waste. Some powders, such as beryllium, require the application of heat

as well as pressure to achieve full density. Likewise, complicated shapes require isostatic pressing. Thus, there is a growing need for the fast, efficient use of hot isostatic pressing (HIPing). Unfortunately, HIPing is neither fast nor inexpensive. The expense of HIPing combined with the expense and environmental hazards associated with many powders precludes the use of the once common practice of recursive die tooling and HIP schedule modification until a part achieves a near-net shape. Overcoming these difficulties requires modeling.

One common approach to solving these problems lies in the micromechanical modeling method first introduced by Ashby [1972] and further discussed in Artz [1983]. This model assumes a random dense packing of monosized spheres that, when subjected to heat and pressure, densify according to the mechanisms of plastic yielding, diffusion, and creep. The utility of such a model is exemplified in the generation of HIP densification maps which show the density achieved by a powder compact under specific conditions along with the corresponding amount of grain growth and the primary densification mechanism involved. Numerous authors are using the micromechanical model as a guide to more efficient HIP processing of complex shapes [Bingert *et al.*, 1997; Suryanarayanan *et al.*, 1993, 1994].

Unfortunately, there are a number of limitations to the micromechanical modeling procedure. The most obvious is that the quality of the model is limited to the quality of the input data. Another important point is that the quality of the model is influenced more by one parameter than another and it is important to know ahead of time which parameters are most influential as it will be these that are the greatest source of error. Thirdly, the consolidation properties of a powder used in published

densification work may be considerably different than those of the powder with which a researcher is working. These differences arise from differences in surface chemistries, formation methods (attrition vs. atomization), particle size distributions, and morphologies. There has been a significant amount of work into sensitivity analysis of input parameters for the micromechanical model [Suryanarayanan *et al.*, 1993]. These authors point out that in terms of the densification rate for metals, it is the power law creep mechanisms that are most influential and thus the most important parameters are the yield stress, power law creep reference stress, and power law creep exponent. It should be noted, however, that most tuning of the micromechanical model parameters is done based on experimental densification data alone and not on grain growth or dominate densification mechanism data, both of which can be obtained from proper microstructural analysis. This is an important point to consider when optimizing parameters since different parameters may fit the densification data equally well but will result in different dominant densification mechanisms and grain growth maps.

An improvement in the micromechanical modeling methods would result in a drastically better understanding of the temperature and pressure schedules needed to achieve full density while at the same time minimizing grain growth. This in turn would save time, materials costs, retooling costs, finishing costs, and environment/worker exposure. This paper presents the results of using a fuzzy logic based multiobjective genetic algorithm to optimize the parameters of copper powder as studied by Wadley *et al.* [1991]. The fuzzy logic based multiobjective genetic algorithm methodology was

presented elsewhere [Reardon, 1997a, 1997b]. A brief description follows in the next section.

The problem at hand is taken from the third tutorial of Ashby's HIP 6.0 Background Reading [Ashby, 1990] with a few modifications. The main modification being that in this optimization the micromechanical densification rate equations as well as the grain growth rate equations are solved numerically as a function of time. This results in considerably less accumulation of error than in the numerical solution as a funciton of density used by Ashby and Artz in the calculation of densification maps. Since the solving of the equations occurs in two fundamentally different ways between the present study and Ashby's HIP6.1 (Ashby, 1987), the optimized parameters from this work will not necessarily appear to be most optimal when inserted into HIP 6.1.

1.2 Nonlinear curve fitting

Generally speaking, one can formulate any optimization problem into a single standard of measurement - a cost function or a fitness function - that determines the performance of a decision and then recursively improves the performance by selecting from the most feasible of alternatives. A typical scenario in nonlinear parameter optimization would involve minimizing the least squares difference between all the data points of a calculated and experimental densification curve (density v. temperature or density v. pressure). In other words, to minimize the quantity:

$$\Phi = \frac{1}{N}\sum_{i=1}^{N}\left(\rho_{Ei} - \rho_{Ci}\right)^2, \qquad \text{Eq. 1.}$$

where N is the number of data points, ρ_{Ei} is an experimental data point, and ρ_{Ci} the calculated densification point. Traditional deterministic optimization techniques require the use of gradient or higher order statistical analysis of Φ:

$$\frac{\partial \Phi}{\partial a} = \frac{2}{N}\sum_{i=1}^{N}\left(\rho_{Ei} - \rho_{Ci}\right)\frac{\partial \rho_{Ci}}{\partial a} = 0 \qquad \text{Eq. 2.}$$

for each variable, *a*, being optimized.

Such an approach can only handle the optimization of one densification curve at a time and typically does not properly account for the uncertainty that is inevitably present in the experimental data. To complicate matters, complete densification curves are not always readily available. Instead, individual density points at various temperatures and pressures are usually the most common form of densification data.

The fuzzy logic based multiobjective genetic algorithm (GA), as described in previous papers [Reardon, 1997a; 1997b], is ideally suited to overcoming these deficiencies. First, the GA treats each individual data point as a separate objective to which the model parameters must be optimized and thus there is no need for smooth experimental densification curves. Second, there is no limit to the number of objectives or parameters that can be operated on at one time. Third, the use of fuzzy rule sets to determine the most optimal of parameters allows for one to incorporate experimental error.

1.3 The Genetic Algorithm

Darwinian evolution is an intrinsically robust search and optimization procedure. Evolved biota have optimized solutions to complex problems at every level of organization, from the cell up to the population. The problems that biota have solved and continue to improve upon, are typified by chaos, chance, temporality, nonlinearity, and multidimensionality. Such problems have proven to be intractable to deterministic optimization techniques, especially in situations where heuristic solutions are not available.

A GA falls into the much broader category of evolutionary algorithms. These algorithms attempt to simulate the processes of evolved biota in optimization. The essence of such a simulation lies in the expression of a solution to a problem not as a single value but as a string of fundamental building blocks (genes) that can be manipulated in much the same way as an extant species will manipulate its gene pool through selection and mating to produce more optimal offspring for the current environment. For example, consider x_1, which is a member of a population of feasible solutions to a problem but not necessarily the optimal solution. The real value of x_1 is expressed as a string of binary digits, e.g.: 101101110. This binary string is mapped to a real value of x_1 such that the string 11111111 corresponds to x_{max} and 00000000 corresponds to x_{min}. x_{max} and x_{min} define the upper and lower bounds respectively of the range of x that is being searched. The real value of x_1 is commonly referred to as a phenotype. If a function requires the optimization of more than one variable, $f(x,y)$, then the total string for a specific member is formed by placing the binary digits

defining *x* and *y* back to back in one string. For example if x_1=001100 and y_1 = 110001 then the string for member #1 would be: 001100110001.

Manipulation of these strings occurs in much the same way as extant species manipulate chromosomes. First, competition among members of the population determines who is most fit or optimal. Second, the most optimal members are allowed to reproduce. Reproduction involves slicing the chromosomes of two members of the populations and then exchanging the segments:

$$\begin{array}{l} X_1 : 10100011 \\ X_2 : \underline{11110111} \end{array} \rightarrow \begin{array}{l} \tilde{x}_1 : 1010\underline{0111} \\ \tilde{x}_2 : \underline{1111}0011 \end{array}$$

$\tilde{x}_1$ and $\tilde{x}_2$ are the resulting progeny and will be placed in the next generation. The actual crossover site is selected randomly with some probability, p_c. Third, mutation occurs, which in a positively entropic system ensures genetic diversity in the subsequent generation. Mutation involves flipping the value of a randomly selected bit with some probability, p_m. The new population that evolves from the selection, crossover, and mutation operators is defined as a generation. This cycle is repeated for a number of generations as specified by the user.

Multiobjective optimization using fuzzy logic can be summarized in two steps. First, a single fitness value that incorporates the values of all the objectives is calculated using fuzzy rule sets. Second, two randomly selected members are compared to a comparison set. If one member has a fuzzy fitness value that

dominates the set and the other does not then the dominating member is selected. Otherwise, continuously updated phenotypic niching is incorporated.

The key to the fuzzy logic approach lies in the definition of the fitness function and its corresponding fuzzy rules:

$$F = \frac{1}{N}\sum_{i=1}^{N} f'\left(f_i\right) \qquad \text{Eq. 3}$$

which is essentially an average over the N objectives in question. *f'* is a fuzzy logic rule set that scales the objective, f_i, according to how far away it is from the experimentally optimal solution. A typical fuzzy set would have the form:

$$\text{if } f_i \le \left(O_i - E_i\right) \rightarrow f'\left(f_i\right) = \left(\frac{S_{\min}}{f_{i\min} - \left(O_i - E_i\right)}\right)\left(f_i - \left(O_i - E_i\right)\right) \qquad \text{Eq. 4a}$$

$$\text{if } \left(O_i - E_i\right) \le f_i \le \left(O_i + E_i\right) \rightarrow f'\left(f_i\right) = 0 \qquad \text{Eq. 4b}$$

$$\text{if } f_i \ge \left(O_i + E_i\right) \rightarrow f'\left(f_i\right) = \left(\frac{-S_{\max}}{\left(O_i + E_i\right) - f_{i\max}}\right)\left(f_i - \left(O_i + E_i\right)\right) \qquad \text{Eq. 4c}$$

where O_i is the ith experimental value that the ith function, f_i, is being optimized towards, E_i is the error or accepted uncertainty in O_i, $S_{min(max)}$ is a scaling parameter for values below (above) the accepted value, $f_{imin(imax)}$ is the smallest (largest) value of all the *i*th objectives in the population.

1.4 Defining the upper and lower bounds of the search space

The efficiency of all optimization techniques is greatly enhanced when reasonable limits are placed on the search space. The fuzzy logic based GA is no exception and to that end, the Ashby's HIP Users Manual [Ashby, 1990b] and references therein provides limits for all of the parameters to be optimized.

1.5 Densification curve sensitivity to parameter values

The stochastic nature and large population size of a fuzzy logic based multiobjective GA provides a distribution of feasible answers to a problem. Thus, parameters that are not very important (i.e.: do not have a significant impact on the objective values will have a broad, almost random, distribution and parameters that do significantly impact the objective values will have a narrow distribution.

Thus, the final optimized population provided by a GA provides insight to the sensitivity of the parameters on the models. Formal sensitivity analysis has been conducted previously [Suryanarayanan *et al.*, 1993, 1994]. This work reveals that in many metals, such as that of copper powder, the yield stress and the parameters of the power law creep mechanism are the most influential factors in the densification model. Thus, if the fuzzy logic based GA operates as expected, the optimized population will show these parameters to have a narrow distribution and the other parameters to have a much broader or random distribution.

2.0 Procedure

The first step in fuzzy logic based GA optimization, is to determine the parameter range to be searched. Table I lists the range for each parameter. Before initiating the optimization routine, the upper and lower bounds are tested in Ashby's HIP 6.1 model and compared to the experimental data to ensure that the test bounds contain the optimal solution. Figure 1 shows the results of the upper and lower limits in a typical density v. pressure and density v. temperature plot with Wadley *et al.*'s [1991] data.

The second step is defining the objectives to be optimized. In this work, the goal is to minimize the difference between the calculated densification values and the six data points of Wadley *et al.*'s [1991] work within a specified experimental error. The actual experimental error was not available in the original paper and thus it had to be approximated. Table II lists the objective conditions of Wadley et al's [1991] six data points along with experimental error estimated by the present author. Note that the GA will only calculate the densification data for these points and not the entire densification map. The density is calculated as a function of time, temperature and pressure. For all six data points, the temperature and pressure are ramped up from ambient conditions to the values in Table II over a period of 15000 seconds after which the temperature and pressure are held constant for the remainder of the experimental time frame. This procedure was followed to ensure a minimum accumulation of error in the densification rate equations.

The third step is to define parameters of the GA itself. Table III lists the parameters of the GA used in this optimization.

3.0 Results and Discussion

The stochastic nature of a GA optimization requires multiple runs to ensure reproducibility. Thus, for this work, the GA was run four times and each time similar results were obtained. Figures 2a and 2b show the fitness averaged over the entire population and the associated standard deviation of the averages for two of the six objective functions. All of the objective functions behaved in a similar fashion in that their absolute values were minimized and the standard deviation decreased with generation number indicating convergence.

The model parameters being optimized also behaved in a similar manner from run to run. Figure 3a and 3b shows the evolution of two of the16 parameters. While the power law creep reference stress is clearly converging to a specific value, as indicated by the standard deviation, the surface energy is not. This behavior is to be expected as the densification model is known to be more sensitive to some parameters, such as the power law creep reference stress, than to others.

Once the optimization is complete, a member of the population can be selected based on its ability to minimize the objective functions to be used in the micromechanical model. Table IV lists a few member's parameter values and the associated objective values produced after the 20th generation. A mulitobjective optimization technique such as this finds a distribution of feasible solutions to a problem. Thus, with the exception of an occasional member who is clearly not optimal due to a random mutation, all of the remaining members are optimal. In other words, though the members may have different parameter values, they all solve the problem

as defined and thus no one member is better fit than any of the others. This fact is well shown in Table IV where many different parameter values result in acceptable objective values. Figure 4 shows how the five members in Table IV provide similar relative densities after 30000s but the path taken by each one is different. This fact would indicate that more experimental information on the densification path is needed to properly optimize the parameters.

As indicated in Figures 3a-b, the parameters are optimized in an equally efficient manor. Table V lists the average parameter value and associated standard deviations after 25 generations. When the standard deviations are normalized with respect to the parameter search space range and the inverse of the normalization is taken one obtains a measure of how sensitive the model is to the parameter in question. Thus, from Table V, one can assume that the yield stress, the power law creep reference stress and the activation energy for boundary diffusion are the most important factors in accurately modeling the densification maps. This result is in broad agreement with Suryanarayanan *et al.* [1993, 1994].

The work emphasizes an important point when optimizing a large number of parameters (16) with a small number of objectives (6). The point being that there exists a large range of feasible solutions to the problem. Therefore, in order for accurate optimizaiton to take place such that parameter values are determined that give the model predictive cababilities a larger objective data set at more temperatures, pressures, and times is required. Furthermore, a more accurate description of the heat and pressure cycles along with realistic assessments of the experimental uncertainties need to be available for accurate optimization to take place.

Figures 2 and 3 are examples of a common phenomenon in GA's called genetic drift. Figure 3 seems to indicate that the parameter values are converging long after the objective values have converged. This is caused by a number of factors. In a system such as this, with a low mutation rate and a small niche cutoff radius, once the objective values have converged there is no other major selection criteria upon which the GA can base its choices for who is most fit. Thus, faced with a population of equally fit members, selection becomes random and gradually drifts towards one of many optimal values. In this work, while the 50th generation is composed of a few distinct individuals that are highly optimal, it is the earlier generations (20-30) that contain the greatest diversity of equally optimal solutions to the problem.

4.0 Conclusions

A fuzzy logic based multiobjective genetic algorithm, as presented in earlier papers, was used to optimize the micromechanical model parameters of copper powder based on the densification data of Wadley *et al.* [1991]. This procedure determined the optimal values of the16 main parameters as well as the relative impact each parameter has on the final densification model. In addition to showing that the fuzzy logic GA is capable of finding multiple solutions to a multi-objective, multi-variable problem, this work has also shown the importance of having a large objective data set on hand along with a realistic assesment of experimental error and process schedules.

5.0 Acknowledgments

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6.0 References

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6.0 Tables

Table I. Search range for each parameter in the micromechanical model being optimized by the Fuzzy Logic based GA. (PLC: Power Law Creep)

Parameter	Units	Lower Bound	Upper Bound
surface energy	J/m^2	1.0000	2.0000
yield stress	MPa	15.000	200.00
Temperature Dependence of Yield		0.10000	0.90000
PLC Exponent		4.7000	4.9000
PLC Reference Stress	MPa	15.000	200.00
PLC Activation Energy	kJ/mol	150.00	250.00
Low T. to High T. Creep Transition	K	580.00	620.10
C for Low T. Creep		0.50000	0.71000
Pre-exponent for Volume Diffusion	m^2/s	5.0000e-05	7.0000e-05
Activation Energy for Volume Diffusion	kJ/mol	150.00	250.00
Pre-exponent for Boundary Diffusion	m^2/s	4.0000e-15	6.0000e-15
Activation Energy for Boundary Diffusion	kJ/mol	75.000	125.00
Pre-exponent for Surface Diffusion	m^2/s	5.0000e-10	7.0000e-10
Activation Energy for Surface Diffusion	kJ/mol	175.00	225.00
Pre-exponent for Boundary Mobility	m^2/s	4.0000e-15	6.0000e-15
Activation Energy for Boundary Mobility	kJ/mol	100.00	200.00

Table II. The experimental values of copper powder consolidation from Wadley *et al.* used in the optimization.

Time (s)	Temperature (K)	Pressure (MPa)	Relative Density	Est. Error
30000	823.0	25.0	0.970	0.0005
30000	823.0	50.0	0.999	0.0005
30000	823.0	75.0	1.000	0.0005
30000	723.0	50.0	0.953	0.0005
30000	773.0	50.0	0.990	0.0005
30000	823.0	50.0	0.999	0.0005

Table III. The GA parameters used in the optimization.

Binary string length for each variable	14
Number of generations per optimization	50
Population size	300
Mutation Probability	0.1%
Crossover Probability	90%
Comparison set Size	1

Table IV. Five example member's parameter values and the associated objective values produced after the 20th generation of the optimization.

	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5
surface energy	1.9690	1.5500	1.5500	1.0190	1.2380
yield stress	27.620	146.20	64.400	23.680	25.110
T. Dep. of Yield	0.66320	0.26560	0.46720	0.27460	0.52700
PLC Exponent	4.8680	4.7170	4.7170	4.8380	4.7590
PLC Ref. Stress	53.300	25.670	25.670	45.290	42.860
PLC Act, Engy	245.30	151.10	151.10	196.30	216.10
Low T. - High T.	580.40	585.90	585.90	611.30	603.10
C for Low T. Creep	0.65590	0.51410	0.51410	0.65300	0.62020
Pre-exp. V. Diff.	5.3650e-5	5.8310e-5	5.8310e-5	5.9620e-5	5.181e-5
Act. Engy V. Diff.	230.40	210.50	210.50	227.20	179.80
Pre-exp. B. Diff.	4.781e-15	5.732e-15	5.732e-15	4.524e-15	4.346e-15
Act. Engy B. Diff.	80.040	82.970	82.970	78.480	79.810
Pre-exp. S. Diff.	5.057e-10	6.598e-10	6.163e-10	5.057e-10	6.891e-10
Act. Engy S. Diff.	211.60	203.70	208.30	199.60	213.10
Pre-exp. B. Mob.	4.201e-15	5.055e-15	5.051e-15	4.97e-15	4.188e-15
Act. Engy B. Mob.	123.70	186.40	199.70	147.90	193.80
Objective 1	2.885e-5	-2.953e-3	-2.953e-3	4.426e-3	3.29e-05
Objective 2	3.636e-5	2.954e-4	2.954e-4	-8.863e-5	2317e-4
Objective 3	-1.013e-6	-1.550e-5	-1.550e-5	0.0	0.0
Objective 4	4.789e-4	9.326e-4	9.326e-4	6.097e-3	2.687e-3
Objective 5	-7.014e-3	-1.039e-3	-1.039e-3	-4.072e-3	-4.755e-3
Objective 6	3.636e-5	2.954e-4	2.954e-4	-8.863e-5	2.317e-4

Table V. The average parameter value and associated standard deviations after 25 generations along with the resulting degree of sensitivity the objective has to each parameter..

Parameter	$\bar{x}$	σ_x	$\frac{(x_{max} - x_{min})}{\sigma_x}$
surface energy	1.2930	0.23840	4.1946
yield stress	35.710	22.580	8.1931
T. Dependence of Yield	0.44520	0.21520	3.7175
PLC Exponent	4.8280	0.048650	4.1110
PLC Reference Stress	50.910	17.980	10.289
PLC Activation Energy	211.00	16.520	6.0533
Low T. to High T. Trans.	606.50	7.6000	5.2763
C for Low T. Creep	0.60040	0.044170	4.7544
Pre-exp. for V. Diff.	5.9870e-05	4.1480e-06	4.8216
Act. Engy for V. Diff.	212.80	24.950	4.0080
Pre-exp. for B. Diff.	4.4900e-15	3.7040e-16	5.3996
Act. Engy for B. Diff.	79.080	0.68550	72.939
Pre-exp. S. Diff.	6.2160e-10	5.4850e-11	3.6463
Act. Engy S. Diff.	193.00	16.440	3.0414
Pre-exp. B. Mob.	4.9370e-15	5.7590e-16	3.4728
Act. Engy B. Mob.	146.20	31.230	3.2020

7.0 Figures

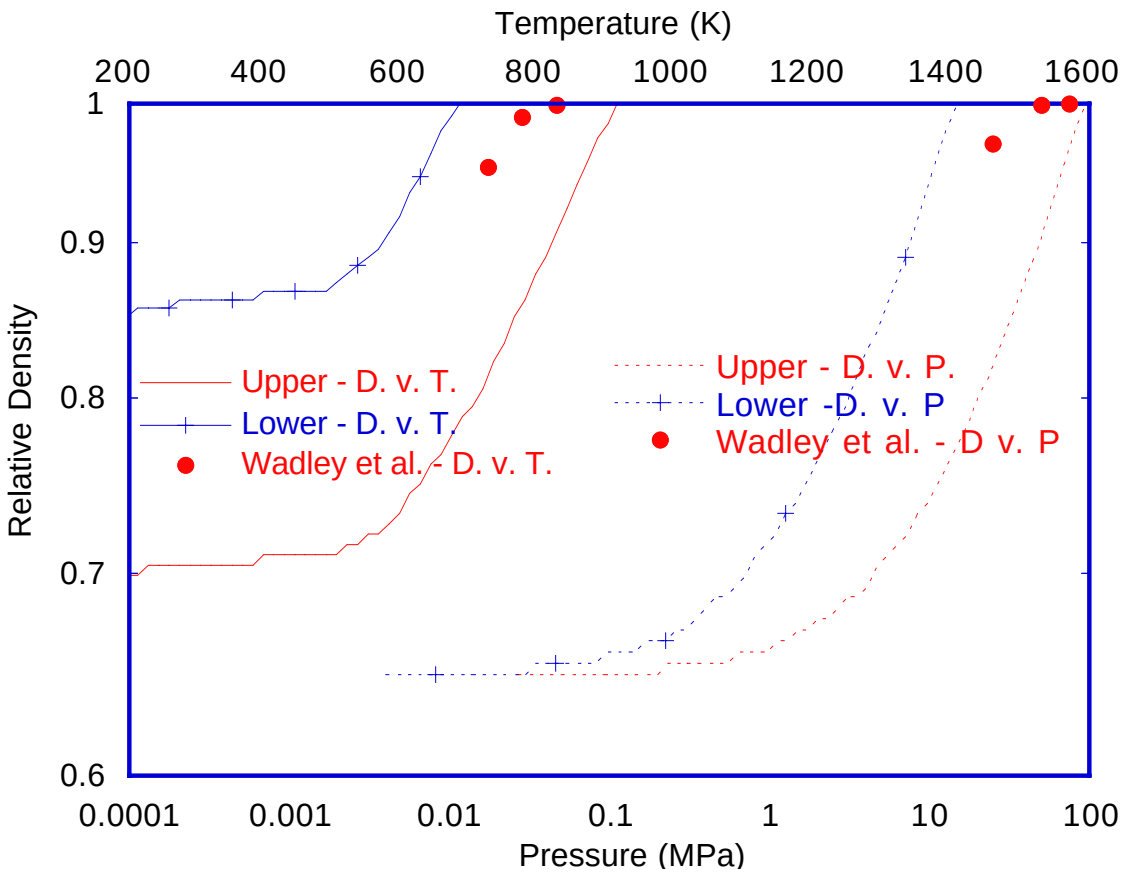
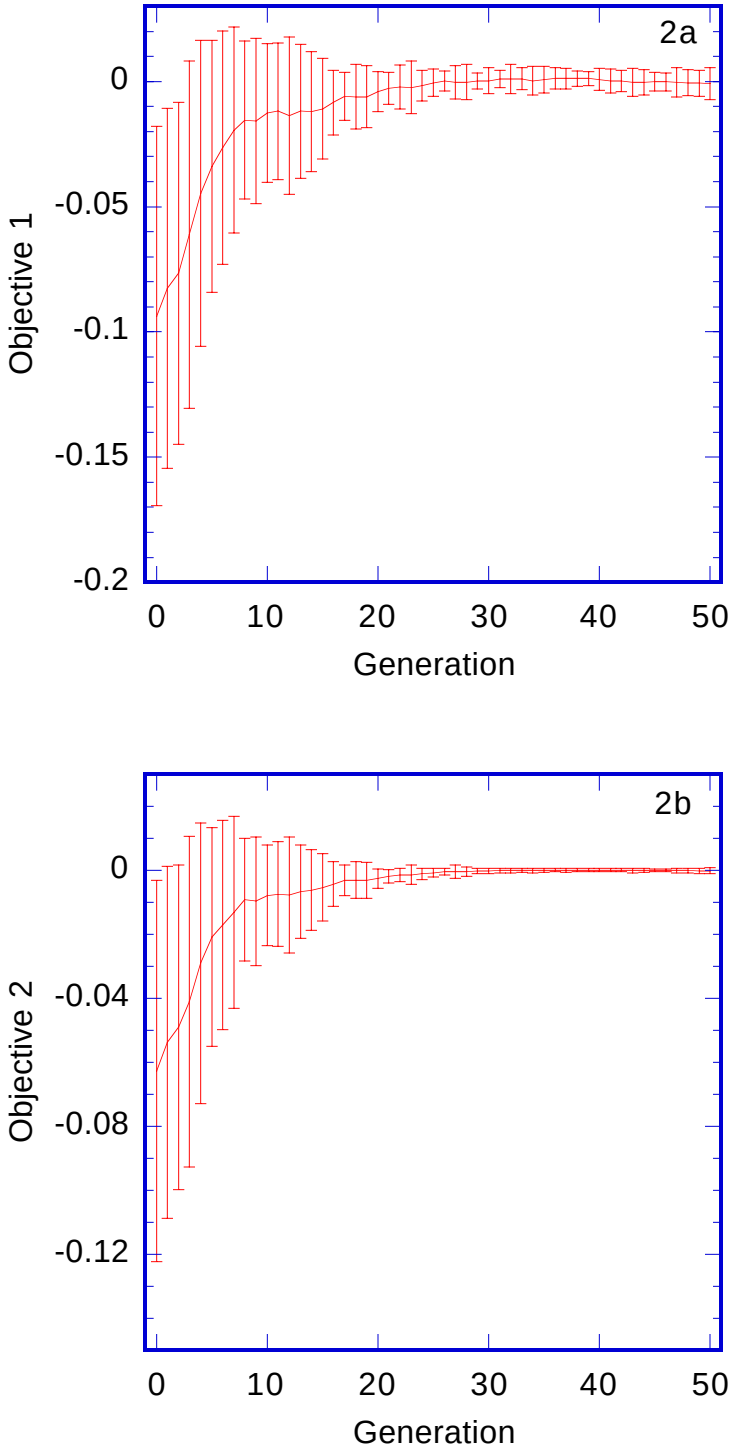


Figure 1. The results of the upper and lower boundary limits in a typical density v. pressure and density v. temperature plot with Wadley *et al.*'s data.



Figures 2a-b. The fitness averaged over the entire population and the associated standard deviation for two of the six objective functions.

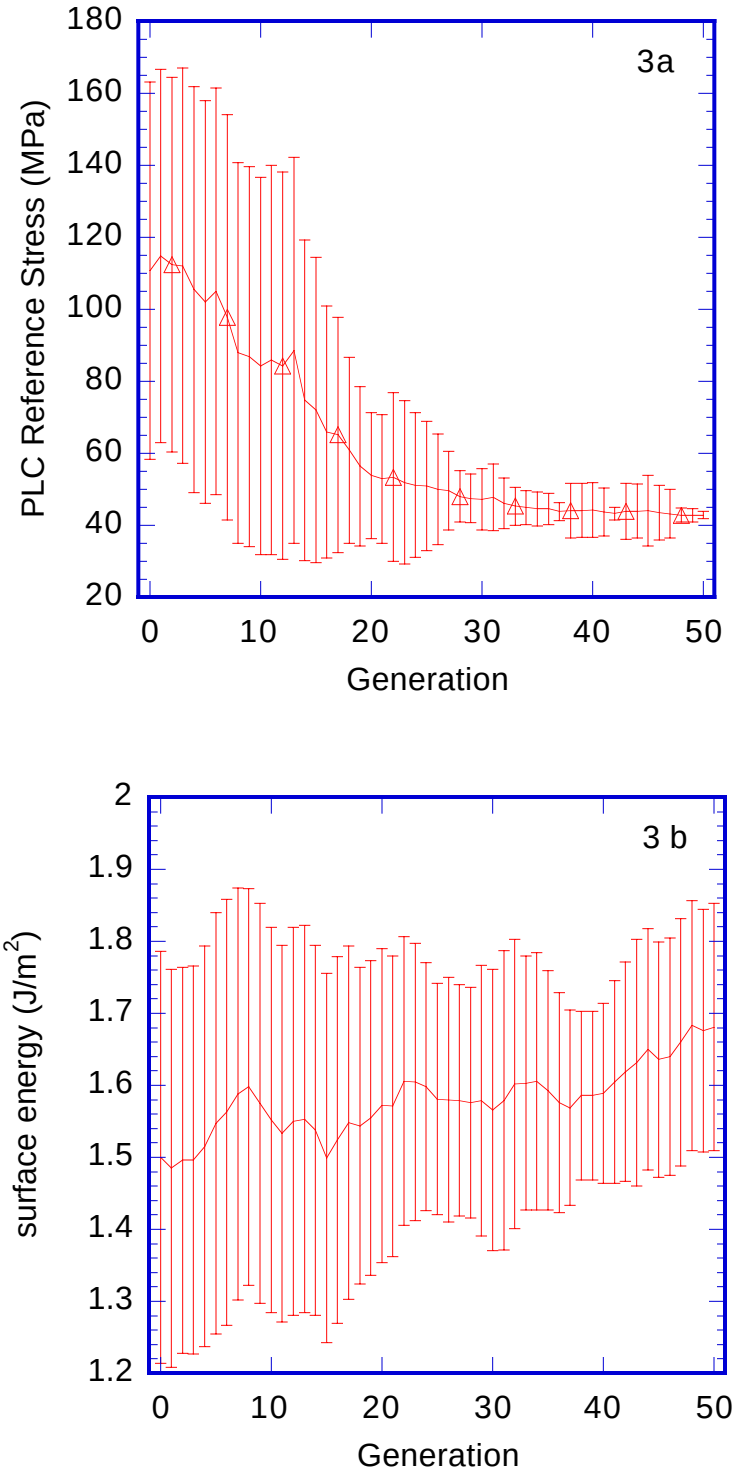


Figure 3a-b. The evolution of the PLC reference stress and the surface energy averaged over the entire population with the associated standard deviations. The PLC stress converges indicating that it is an important parameter where as the surface energy does not, indicating that it is not as significant.

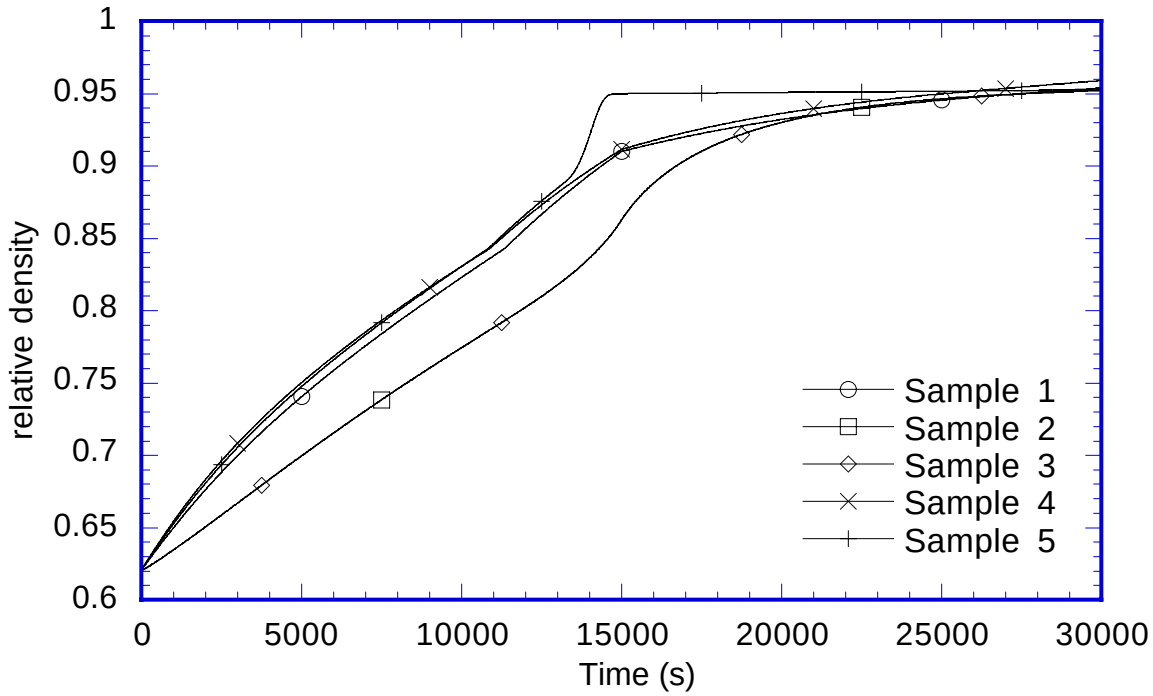


Figure 4. The Relative density v. sintering time for the 5 samples listed in Table IV. This calculation involved a ramping of the temperature and pressure from 0.1MPa and 293K at t=0 to 50MPa and 723K at t=15000. After 15000, the temperature and pressure were held constant. Note that while the final relative density is similar for the samples, the path taken as a funciton of time is different. The apparent discontinuites are due to the smoothing operators between stage 1 and stage 2 densification. As shown here, the smoothing operators work better for some parameter sets than for others.