Title:

ADVANCES IN BERYLLIUM POWDER CONSOLIDATION
SIMULATIONS

CONF-9805118--

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Submitted to:

PROCEEDINGS OF THE 1998 INTERNATIONAL CONFERENCE ON
POWDER METALLURGY AND PARTICULATE MATERIALS,
5/31/98-6/4/98, LAS VEGA, NV.RECEIVED
SEP 22 1998
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ADVANCES IN BERYLLIUM POWDER CONSOLIDATION SIMULATION

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ABSTRACT

A fuzzy logic based multiobjective genetic algorithm (GA) is introduced and the algorithm is used to optimize micromechanical densification modeling parameters for warm isopressed beryllium powder, HIPed copper powder and CIPed/sintered and HIPed tantalum powder. In addition to optimizing the main model parameters using the experimental data points as objective functions, the GA provides a quantitative measure of the sensitivity of the model to each parameter, estimates the mean particle size of the powder, and determines the smoothing factors for the transition between stage 1 and stage 2 densification. While the GA does not provide a sensitivity analysis in the strictest sense, and is 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 BERYLLIUM POWDER PROCESSING

Beryllium and its two most common alloys, beryllium-copper and beryllium-aluminum have a number of interesting properties that make them extremely useful as well as materials of intense study over the past twenty years[1-3]. Unfortunately, the cost and potential hazards[4] of beryllium powder has limited its use to situations in which it is absolutely required. Near net or net shape powder processing has shown to be a viable route around these limitations[3]. However, further development is needed to make the technology competitive. Due to the expense and health considerations involved in this development, computer modeling is a reasonable approach to solving the technological problems at hand.

One common numerical approach to solving these problems lays in the micromechanical modeling method first introduced by Ashby [5] and further discussed by Artz *et al.* [6]. 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 (figure 1.) 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. Many authors are using the micromechanical model as a guide to more efficient HIP processing of complex shapes [7, 8].

Figure 1. HIP densification map for beryllium powder calculated using Ashby's HIP6.1[7].

However, most particle size distributions are not monosized and attritioned particles are not spherical. Thus, in addition to optimizing the 16 main densification parameters, the ideal particle size used in the model must also be optimized.

It should be noted that most tuning of the Ashby HIP 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 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 cost, finishing costs, and environment/worker exposure. This paper presents the results of using a fuzzy logic based multiobjective genetic algorithm to optimize the parameters for HIPed beryllium powder[9], copper powder[10], and tantalum powder[8].

The micromechanical model being used in this optimization differs from Ashby's HIP 6.1 in a number of ways. 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 solutions as a function 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[11], the optimized parameters from this work will not necessarily appear to be most optimal when inserted into HIP6.1.

In Ashby's micromechanical model, densification is expressed as the instantaneous change in density due to particle yielding, $\dot{\rho}_Y$, and the total densification rate, $\dot{\rho}_T$, which is a linear sum of the densification rates due to diffusive mechanisms, $\dot{\rho}_D$, power law creep, $\dot{\rho}_{PLC}$ and Nabarro-Herring creep, $\dot{\rho}_{NH}$. For densities less than ρ_1 , which is considered to be an adjustable parameter, the densification equations are:

$$\dot{\rho}_Y = \left[\frac{P(1-\rho_o)}{1.3\sigma_Y} + \rho_o^3 \right]^{1/3} \quad \text{Eq. 1.}$$

where P is applied pressure, σ_Y is yield stress, ρ_o is the initial density;

$$\dot{\rho}_D = 32(1-\rho_o) \frac{D_V}{r^2} \tilde{F}_1 + 43 \frac{(1-\rho_o)}{(\rho-\rho_o)} \frac{\delta D_B}{r^3} \tilde{F}_1 \quad \text{Eq. 2.}$$

where r is the particle radius, ρ is the present density, δ is the grain boundary width;

$$\dot{\rho}_{PLC} = 3.1\rho \left[\frac{(1-\rho_o)}{(\rho-\rho_o)} \right]^{1/2} D_c \left[\left[\frac{(1-\rho_o)}{(\rho-\rho_o)} \right] \left[\frac{P-P_o}{3\rho^2\sigma_{REF}} \right] \right]^n \quad \text{Eq. 3.}$$

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 not equally influenced by all parameters and it is important to know *a priori* which parameters are most influential as it will be these that are the greatest source of error. Next, the sintering parameters of a powder used in published densification work may be considerably different than those of the powder with which a researcher is working and thus each researcher must be able to optimize the model parameters base on their own densification data. These differences in powders arise from differences in surface chemistries, attrition vs. spray forming, size distributions, and morphologies. Finally, the standard micro-mechanical models assume a random dense packing of monosized spheres.

where σ_{REF} is the power law creep reference stress, n is the power law creep exponent, P_o is the initial internal pore pressure;

$$\dot{\rho}_{NH} = \frac{14.4}{\rho} \left[\frac{(1-\rho_o)}{(\rho-\rho_o)} \right]^{1/2} \left[\frac{D_V}{G^2} + \frac{\pi\delta D_B}{G^3} \right] \tilde{F}_1 \quad \text{Eq. 4.}$$

where G is the grain size;

$$\tilde{F}_1 = \frac{(P-P_o)\Omega}{kT} + \frac{3\rho^2(2\rho-\rho_o)\gamma\Omega}{(1-\rho_o)rkT} \quad \text{Eq. 5.}$$

where k is Boltzman's constant, T is temperature, γ is surface energy, Ω is atomic volume;

$$D_V = D_{OV} \exp\left(\frac{-Q_V}{RT}\right) \quad \text{Eq. 6.}$$

where D_{OV} is the volume diffusion pre-exponential factor, Q_V the volume diffusion activation energy, R is the gas constant;

$$D_B = D_{OB} \exp\left(\frac{-Q_B}{RT}\right) \quad \text{Eq. 7.}$$

where D_{OB} is the boundary diffusion pre-exponential factor, Q_B the boundary diffusion activation energy;

$$D_C = 10^{-6} \exp\left(\frac{-Q_C}{RT_M} \left(\frac{T_M}{T} - 2\right)\right) \quad \text{Eq. 8.}$$

where T_M is the melting temperature, Q_C the power law creep activation energy.

For densities greater than ρ_2 which is also considered to be an adjustable parameter the densification rate equations are:

$$\rho_Y = 1 - \exp\left[\frac{3P}{2\sigma_Y}\right] \quad \text{Eq. 9.}$$

$$\dot{\rho}_D = 3 \left[\frac{1-\rho}{6\rho} \right]^{1/3} \frac{D_V}{r^2} \tilde{F}_2 + 4 \frac{\delta D_B}{r^3} \tilde{F}_2 \quad \text{Eq. 10.}$$

$$\dot{\rho}_{PLC} = 1.5\rho(1-\rho)D_C \left[\frac{1.5(P-P_1)}{n\sigma_{REF}(1-(1-\rho)^{1/n})} \right]^n \quad \text{Eq. 11.}$$

$$\dot{\rho}_{NH} = 32(1-\rho) \left[\frac{D_V}{G^2} + \frac{\pi\delta D_B}{G^3} \right] \tilde{F}_2 \quad \text{Eq. 12.}$$

$$\tilde{F}_2 = \frac{(P-P_1)\Omega}{kT} + \frac{2\gamma\Omega}{rkT} \left[\frac{6\rho}{1-\rho} \right]^{1/3} \quad \text{Eq. 13.}$$

$$P_1 = \left[\frac{1-\rho_c}{1-\rho} \right] \frac{\rho}{\rho_c} P_o \quad \text{Eq. 14.}$$

where ρ_c is the critical density at which pores become closed. For densities falling between ρ_1 and ρ_2 the above equations (2-4 and 10-12) are scaled accordingly and summed to give the total densification rate.

In this work, all of the adjustable parameters listed in Table I will be optimized such that the difference in the calculated and experimental density points is minimized.

Table I. Search range for each parameter in the micromechanical model being optimized by the Fuzzy Logic based GA. The lower and upper bounds listed are for the beryllium powder study. (PLC: Power Law Creep)

Parameter	Units	Lower	Upper
surface energy	J/m ²	1.5	2.5
yield stress	MPa	10	1500
Temp. Dependence of Yield		0.1	2.7
PLC Exponent		5	12
PLC Reference Stress	MPa	1900	2600
PLC Act. Energy	kJ/mol	900	1300
Low T. - High T. Creep Trans.	K	500	800
C for Low T. Creep		0.5	0.71
Pre-exponent Vol. Diff.	m ² /s	1e-5	3e-5
Act. Energy Vol. Diff.	kJ/mol	110	400
Pre-exponent Boundary Diff.	m ² /s	3e-15	5e-15
Act. Energy Boundary Diff.	kJ/mol	75	125
Pre-exp. Surface Diff.	m ² /s	1.1e-12	2e-10
Act. Energy Surface Diff.	kJ/mol	110	250
Pre-exp. Boundary Mob.	m ² /s	1e-15	3e-15
Act. Energy Boundary Mob.	kJ/mol	100	200
Particle size Radius	m	2e-5	3.5e-5
Stage 2 cut off relative density		0.7	0.99
Stage 1 cut off relative density		0.7	0.99

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 vs. temperature or density vs. pressure). In other words, to minimize the quantity:

$$\Phi = \left| \frac{1}{N} \sum_{i=1}^N (\rho_{Ei} - \rho_{Ci})^2 \right|, \text{Eq. 15.}$$

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 :

$$\frac{\partial \Phi}{\partial a} = \frac{2}{N} \sum_{i=1}^N (\rho_{Ei} - \rho_{Ci}) \frac{\partial \rho_{Ci}}{\partial a} = 0 \quad \text{Eq. 16.}$$

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 GA, as described in previous papers [12-15], 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 and to estimate how the experimental error would broaden the range of optimal parameter values.

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 ecosystem. 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. Consider the problem of figure 2 where the goal is to find the value of x which minimizes both $f(x) = x^2$ and $f(x) = (x-2)^2$. A GA quantizes the search range into 2^L different regions and assigns each region a distinct binary code or chromosome that is L digits (alleles) long. The actual binary structure of a chromosome is called the genotype whereas the real value of x that the binary string is mapped to is the phenotype. The GA then randomly selects a subset of these chromosomes. Each selected chromosome constitutes a member of the initial population.

Figure 2. A GA quantizes a search range into 2^L ($L=4$) different segments. Each segment is associated with a binary string that is directly convertible to a real value of x .

This particular problem is an excellent example of a multiobjective problem in which the objectives are in conflict. There is no single value of x which minimizes both functions, thus the GA locates the region which provides the best of all possible solutions. Many engineering problems fall into this general category of problems. For example, process design problems such as HIPing schedules often involve conflicting objectives where one wants to maximize densification but minimize grain growth, process time, temperature, and pressure. Furthermore, model optimization often requires that calculated quantities be compared to experimental quantities which inevitably contain some degree of uncertainty. Knowing to what degree this uncertainty effects the breadth of optimal parameter values of one's model is important in determining which model parameters are most influential and thus the optimization routine used must be able to determine optimal parameter ranges. As shown in figures 3a-c, the GA is clearly able to fulfill this requirement.

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:

$$X_1 : 1000 \quad \bar{X}_1 : 1001$$

$$X_2 : 1101 \quad \bar{X}_2 : 1100$$

$\bar{X}_1$ and $\bar{X}_2$ 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 allele 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.

Figures 3a-c shows the evolution of a population towards the optimal solution of the problem discussed in figure 2 where $L=14$. After 20 generations, the population evolves towards the optimal region for this problem, $0 \leq x \leq 2$.

Figures 3a-c. a) The initial population, generation 0. b) The population evolved 5 generations. c) The population distribution as a function of generation up to 20 generations.

The theoretical underpinnings of the mechanics of a GA and the kinds of problems it is most adept at solving is outlined in Goldberg [16]. However, for the sake of clarity, a brief discussion will

be provided here. The binary chromosomes of figure 2 can be broken down into fundamental building blocks called schemata. For example, the string 1***, where the * is a wild card, is one particular schema whereas *1*0 and 1111 are two others. Each schema covers a specific area of the search range so that the 1*** covers the range from $0 \leq x \leq 6$ and the ***1 covers every other segment of the 24 present in figure 2. from -6 to 6. Thus, each schema has its own average fitness. Viewed in this way, it becomes apparent that the evaluation of one particular member of the population with a chromosome length of L is equivalent to a statistical sampling the function in question in 2^L distinct regions of the search space because one chromosome necessarily contains 2^L distinct schemata. Consequently, the evaluation of an entire population of size n results in the processing and analysis of 2^L to $n2^L$ different regions of the search space. In the example of figures 3a-c, $n=30$ and $L=14$. Thus, the evaluation of one value of x elucidates information on 16,384 regions of the search range and the processing of each generation covers between 16,384 and 491,520 different regions. This *implicit* parallelism in the evaluation of the search range is the source of the GA's trenchantness.

The example of figure 2 and many practical engineering problems involve multiple conflicting objectives. In a single objective problem it is trivial to determine which member is better fit. However, in multiobjective problems this evaluation can be complex. While many approaches to determining fitness in a multiobjective landscape have been proposed [see [12] for a review], even the highly effective Niched-Pareto[17] method has shortcomings [12, 13]. By incorporating fuzzy logic into the selection procedure, many of these shortcomings are ameliorated [12-15]

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. This means that a member is deemed more fit not on its ability to solve the problem but on its level of phenotypic uniqueness in the partially filled next generation.

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

$$F = \frac{1}{N} \sum_{i=1}^N f'(f_i) \quad \text{Eq. 17.}$$

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:

$$\text{if } f_i \leq (O_i - E_i) \rightarrow f'(f_i) = \left(\frac{S_{\min}}{f_{i\min} - (O_i - E_i)} \right) (f_i - (O_i - E_i)) \quad \text{Eq. 18a.}$$

$$\text{if } (O_i - E_i) \leq f_i \leq (O_i + E_i) \rightarrow f'(f_i) = 0 \quad \text{Eq. 18b.}$$

$$\text{if } f_i \geq (O_i + E_i) \rightarrow f'(f_i) = \left(\frac{-S_{\max}}{(O_i + E_i) - f_{i\max}} \right) (f_i - (O_i + E_i)) \quad \text{Eq. 18c.}$$

where O_i is the i th experimental value that the i th 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 this work $S_{\min(\max)} = 1$) for values below (above) the accepted value, $f_{i\min(i\max)}$ 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 [18] 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 insignificant will have a broad, almost random, distribution and parameters that do significantly impact the objective values will have a narrow distribution. Therefore, 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 [19]. However, this work did not focus on actual optimization of the model parameters.

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. In addition to the densification mechanism parameters themselves, the fuzzy logic GA will also be optimizing the particle size and the smoothing parameters that control the transition between stage 1 and stage 2 densification.

The smoothing functions operate in the following way: If the current density, ρ , $\leq$ the stage 2 cut off density, ρ_2 , then the stage 1 and stage 2 weighting factors (s_1 , s_2) are 1 and 0 respectively. If $\rho \geq$ the stage 1 cut off density, ρ_1 , then $s_1=0$ and $s_2=1$. If $\rho_2 \leq \rho \leq \rho_1$, then $s_1=(\rho_1-\rho)/(\rho_1-\rho_2)$ and $s_2=1-s_1$. All of the appropriately weighted densification rates are then added to give a total densification rate.

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 densification data points of each of the several experimental studies available within a specified experimental error. The actual experimental error was not available in any of the original work and thus it had to be approximated.

Table II. The experimental values of warm isopressed Beryllium powder consolidation from Roberts [9] used in the optimization. The optimization assumes a 500s ramp up from 293K and 0.1 MPa, a 3600s hold, and a 500s ramp down to ambient temperature and pressure.

Time (s)	T (K)	P (MPa)	Rel. Den.	Est. Error
3600.0	873	0.1	0.78	0.005
3600.0	873	55.158	0.81	0.005
3600.0	873	82.737	0.91	0.005
3600.0	923	0.1	0.78	0.005
3600.0	923	15.168	0.80	0.005
3600.0	923	38.611	0.84	0.005
3600.0	948	0.1	0.78	0.005
3600.0	948	31.026	0.80	0.005
3600.0	948	42.058	0.92	0.005
3600.0	948	48.267	0.95	0.005
3600.0	973	0.1	0.78	0.005
3600.0	973	6.895	0.80	0.005
3600.0	973	14.479	0.83	0.005
3600.0	973	15.168	0.84	0.005
3600.0	973	27.579	0.90	0.005
3600.0	973	38.611	0.91	0.005
3600.0	973	55.158	0.97	0.005

Table II lists the objective conditions of the data set 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. Also, the exact heating and pressure schedules were not available in Roberts' [9] report. Thus, it was assumed that the temperature and pressure were ramped over 500s to the temperatures and pressures reported by Roberts and then held for 1 hour.

The third step is to define parameters of the GA itself. In this work, $L=14$, $p_m=0.001$, $p_c=0.9$, and the population size for the beryllium study was 300 whereas for the copper and tantalum studies the population size was 100.

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 4a and 4b show the fitness averaged over the entire population and the associated standard deviation for two objective functions from Roberts' data set. 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. As indicated in figures 4a and 4b some of the objectives were minimized to zero whereas others were minimized to a value other than zero. Furthermore, as indicated by the standard deviation in figure 4b, there were members of the population that solved the objective well in early generations but the GA eventually evolved towards solutions that were less optimal. The reason for this lays in the fact that all of the objectives were being optimized simultaneously. Thus, while a member in an early

generation of figure 3b may have been optimal in solving one particular objective, it was not optimal in solving all of the objectives in question. The mandate of the fuzzy logic based multiobjective GA is to find the best of all possible tradeoffs between all the objectives in question and thus, for the objective in figure 4b, a slightly less than optimal solution satisfies that mandate. The final convergence of the population towards an objective value that was clearly not as optimal in figure 4b as in other objectives results from one of two conditions. First, the model may be lacking in its ability to properly simulate the densification mechanisms of this powder at this density, time, pressure and temperature. Second, the experimental error, which was not reported by Roberts, may be large enough to encompass the calculated value within one standard deviation.

Figures 4a-b. The fitness averaged over the entire population and the associated standard deviation for two of the sixteen objective functions.

The model parameters being optimized behave in a similar manner from run to run. Figures 5a and 5b show the evolution of two of the 19 parameters (16 model parameters, the particle size, and 2 cutoff densities) while optimizing with Roberts' data set. As is typical of metal powders, the yield stress and power law creep mechanisms seem to be the most sensitive parameters and thus tend to converge most quickly. Other parameters, such as the surface energy, however, do not converge quickly because they do not have a significant impact on the model.

Figure 5a-b. The evolution of the yield stress and the surface energy averaged over the entire population with the associated standard deviations. The yield stress converges indicating that it is an important parameter whereas the surface energy does not, indicating that it is not as significant.

Table III. The average parameter values and 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	2.0050	0.19990	5.0025
yield stress	968.50	44.500	33.483
T. Dep. of Yield	2.3360	0.13770	18.882
PLC Exponent	8.8440	1.0490	6.6730
PLC Ref. Stress	2208.0	222.40	3.1475
PLC Act. Engy	1149.0	108.70	3.6799
Low T. - High T.	714.60	41.300	7.2639
C for Low T. Creep	0.59280	0.04764	4.4081
Pre-exp. V. Diff.	2.124e-5	6.009e-6	3.3283
Act. Engy V. Diff.	292.30	66.290	4.3747
Pre-exp. B. Diff.	3.839e-15	6.302e-16	3.1736
Act. Engy B. Diff.	108.80	15.730	3.1786
Pre-exp. S. Diff.	8.318e-11	6.471e-11	3.0737
Act. Engy S. Diff.	180.70	39.320	3.5605
Pre-exp. B. Mob.	1.974e-15	6.553e-16	3.0520
Act. Engy B. Mob.	135.50	37.47	2.6688
Particle radius	2.731e-5	4.5e-6	3.3333
stage 2 cutoff den.	0.84310	0.08043	3.6056
stage 1 cutoff den.	0.93690	0.05471	5.3007

parameters indicate that there exists a broad distribution of acceptable solutions to the problem at hand.

Figure 6. The Relative density v. sintering time for 5 optimal members of the population. This calculation involved a ramping of the temperature and pressure from 0.1MPa and 293K at $t=0$ s to 15.168MPa and 973K at $t=500$ s. Holding the temperature and pressure constant for 3600s and then ramping down to ambient conditions in 500s.

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 for the calculation of densification maps. A multitobjective 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 can be considered better fit than any of the others. This fact is shown in Table III where the average parameter values, standard deviations, and sensitivities are listed. The sensitivity parameter is determined by normalizing the parameter search space range with the standard deviation. The rather large standard deviations and low sensitivity of some of the

A cautionary note is in order here. The GA used only the densification data available to optimize the parameters. Thus, while the parameters of interest fit the data present, the rest of the densification and grain growth maps may differ substantially depending on the member of the population that is selected.

Figure 6 shows the relative density vs. sintering time for 5 optimal members of the population. This calculation involved a ramping of the temperature and pressure from 0.1MPa and 293K at $t=0$ to 15.168MPa and 973K within 500s. The temperature and pressure were then held constant for an additional 3600s and then ramped down to ambient conditions in 500s. Even though each member had different parameter values they

produced close to the same final density. Note that the majority of densification occurred in the first 500s of the ramp up phase of the schedule. Since no details of Roberts' original schedule are available (only his hold times), it is possible that different parameter values could have been obtained if a different ramping schedule was used. This ambiguity would then indicate that experimental densification data would be better used if detailed heating and cooling schedules were provided along with the hold times and experimental error.

Table IV. The average parameter values and standard deviations after 25 generations along with the resulting degree of sensitivity the objective has to each parameter for the copper study.

Parameter	$\bar{x}$	σ_x	$\frac{(x_{\max} - x_{\min})}{\sigma_x}$
surface energy	1.2930	0.2384	4.1946
yield stress	35.710	22.580	8.1931
T. Dependence of Yield	0.44520	0.21520	3.7175
PLC Exponent	4.8280	0.04865	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	0.04417	4.7544
Pre-exp. for V. Diff.	5.987e-5	4.148e-6	4.8216
Act. Engy for V. Diff.	212.80	24.950	4.0080
Pre-exp. for B. Diff.	4.49e-15	3.704e-16	5.3996
Act. Engy for B. Diff.	79.080	0.6855	72.939
Pre-exp. S. Diff.	6.216e-10	5.485e-11	3.6463
Act. Engy S. Diff.	193.00	16.44	3.0414
Pre-exp. B. Mob.	4.937e-15	5.759e-16	3.4728
Act. Engy B. Mob.	146.20	31.23	3.2020

recrystallization and dislocation movement upon heating. Likewise, attrition milled powder is notorious for its high BeO content on the particle surfaces. The refractory nature of BeO hinders the diffusion of beryllium and thus increases the effective activation energy of diffusion of the powder. The effects of BeO on the parameters of the micromechanical modeling of beryllium was previously addressed [21]. In Stoev's work, effective diffusion coefficients were developed to account for the hindering effect of BeO on beryllium diffusion. The net result, as implied in the present work, was to decrease the value of diffusion coefficients or increase the activation energy barrier. Thus, without explicitly stating in mathematical terms the effects of a BeO layer on the particles, the GA was able to adjust the available parameters accordingly to create effective activation energies for diffusion through an oxide layer.

The results of a similar copper powder study[14] based on Wadley *et al.*'s work[10] is presented in Table IV and figure 7. The optimization with this particular set of experimental data reveals that power law creep is the major densification mechanism. Also, the differences between the 5 optimal members presented in figure 7 indicate that the exact experimental procedures (ramps up and down) are necessary pieces of information when conducting such an optimization. The experimental uncertainty of Wadley's data was not reported and thus the relative density error window needed by the GA was estimated to be ± 0.0005 .

The tantalum powder data from Bingert *et al.* [8] was also evaluated with the fuzzy logic based GA and the results are presented in Table V. The data in this particular study indicates that diffusion is the main source of densification. This would stand to reason since the samples were CIPed prior to HIPing or sintering. This conclusion is also in agreement with Bingert *et al.* who tuned the parameters manually and found the diffusion parameters to be the most influential mechanisms.

The average physical values and sensitivities of the parameters listed in Table III merit some discussion. According to Table III, the most influential parameters are the yield stress and the temperature dependence of the yield with average values of 970MPa and 2.3 respectively. However, other sources [7, 20] have reported values of 600MPa with a temperature dependence of 1.16. Likewise the activation energies for diffusion found in this optimization are slightly higher than those previously reported. These observations are consistent with the fact that the Roberts' powder was attrition milled. Attrition milled powder is extremely work hardened which would result in a high yield stress and a high temperature dependence of the yield due to an enhanced proclivity towards

4.0 CONCLUSIONS

Figure 7. The Relative density v. sintering time for 5 optimal members of the copper powder consolidation study. 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 15000s, the temperature and pressure were held constant. Note that while the final relative density is similar for the samples, the path taken as a function of time is different. The apparent discontinuities are due to the smoothing operators between stage 1 and stage 2 densification. As shown here, the smoothing operators used in Ashby's original model works better for some parameter sets than for others.

the design of HIP cans so as to more accurately achieve near net or net shape products via HIPing.

Table V. The average parameter values and standard deviations after 50 generations along with the resulting degree of sensitivity the objective has to each parameter for the tantalum study.

Parameter	$\bar{x}$	σ_x	$\frac{(x_{\max} - x_{\min})}{\sigma_x}$
surface energy	2.7567	0.12642	3.9552
yield stress	134.48	2.3860	4.1912
T. Dep. of Yield	0.48020	0.033689	5.9367
PLC Exponent	5.0769	0.41484	7.2317
PLC Ref. Stress	57.139	2.2953	13.070
PLC Act. Engy	481.66	31.262	3.1988
Low T. - High T.	1679.4	23.230	4.3048
C for Low T. Creep	0.63923	0.030731	3.2540
Pre-exp. V. Diff.	6.4724e-3	0.0019201	5.1611
Act. Engy V. Diff.	642.64	58.639	5.1160
Pre-exp. B. Diff.	7.0866e-14	2.428e-14	3.2950
Act. Engy B. Diff.	360.03	47.077	9.5589
Pre-exp. S. Diff.	7.5565e-10	2.8098e-11	3.5590
Act. Engy S. Diff.	411.02	71.331	4.2058
Pre-exp. B. Mob.	1.5103e-14	2.0601e-15	4.8541
Act. Engy B. Mob.	368.99	77.199	3.8861
Particle radius	9.1122e-6	1.0355e-6	2.8973
stage 2 cutoff den.	0.81050	0.04091	4.8888
stage 1 cutoff den.	0.98377	0.011122	13.396

A fuzzy logic based multiobjective genetic algorithm, as presented in earlier papers, was used to optimize the micromechanical model parameters of beryllium, copper, and tantalum powder based on the experimental densification data. This procedure determined the optimal values of the 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 assessment of experimental error and process schedules.

The continuation of this work involves the use of the GA to optimized actual HIP schedules using the optimized Ashby parameters. The main objectives will be to maximize density while minimizing time, temperature, pressure, and grain growth.. Also, there are plans to use the GA in conjunction with an finite element analysis code in

5.0 ACKNOWLEDGMENTS

Funded by the US Department of Energy and Los Alamos National Laboratory which is operated by the University of California under contract number W-7405-ENG-36.

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