Journal of Ceramic Processing Research. Vol. 10, No. 2, pp. 195~201 (2009)

J O U R N A L O F
Ceramic Processing Research

Computer simulation of a ceramics powder compaction process and optimization of process parameters

Y. T. Keum[a,*], J. L. Kim[b] and J. K. Shim[b]

[a]*School of Mechanical Engineering, Hanyang University, 17 Haengdang-dong, Seongdong-ku, Seoul 133-791, South Korea*
[b]*Graduate School of Mechanical Engineering, Hanyang University, 17 Haengdang-dong, Seongdong-ku, Seoul 133-791, South Korea*

In order to optimize the process parameters of ceramic powder compaction, a process simulation was first performed using a finite element method. In the finite element analysis, a quasi-random multi-particle array was introduced for modeling the non-periodic and randomly scattered powder particles with initially-low relative densities. Homogenization theory was employed to find the equivalent material properties associated with various porosities. The size of Al_2O_3 particles, amplitude of the cyclic compaction pressure, and friction coefficient among powder particles were chosen as process parameters. Finite element analysis results show that relative density becomes bigger as the process variables become smaller. Next, a regression model was found by using the response surface method, based on the results of the finite element analysis. Then, the optimal conditions of the process parameters providing the highest relative density were pursued by employing a grid search method.

Key word: Ceramic powder compaction, Homogenization method, Process parameter optimization, Relative density, Response surface method, Grid search method, Finite element analysis.

Introduction

The characteristics of mechanical strength, physical, and chemical properties of poly crystalline ceramic materials are affected by the arrangement of crystal directions because they are caused by the anisotropy of single crystals associated with crystal directions. Therefore, in order to make an analytical model and to perform a computer simulation for a ceramic powder compaction process, it is important to analyze the deformation behavior of material microstructures.

Experimental research on the ceramic powder compaction process has been made in ways to allow the study of the many qualitative characteristics of a poly crystalline ceramic material during the powder compaction process. Even the quantitative analyses of some ideal models are in progress using numerical methods. However, the ideal model of compact forming is different from the real model because the real powders are not regularly arrayed, and the powder density distribution and replenishment state is not uniform. Therefore, to improve the various properties of ceramic components and the efficiency of powder compaction forming processes, the modeling of compaction forming processes, which can quantitatively analyze the real compaction forming process, is recommended. Furthermore, to reduce the time and numerical cost of simulation, the relationship among the relative density and the process parameters influenced greatly by the relative density during the ceramic powder compaction forming has to be considered. In addition, optimal process parameter values for maximizing the relative density should be adopted.

Looking at the research trends of ceramic powder compaction forming, an ideal model in the static and repetitive compactions for compound materials was expedd.

rimentally and numerically studied by Wu *et al*. [1] and Jiang *et al*. [2]. Xin *et al*. [3] introduced a computer simulation method using explicit FEM for analyzing the powder compaction phenomena of single and compound materials. Zahlan *et al*. [4] presented a modeling method for real products made by powder compaction forming under repetitive loads. Zipse [5] also performed research on the FEM simulation of compaction forming and sintering processes of real ceramic products.

Deis and Lannutti [6] and Lu and Lannutti[7-9] measured the density slope and pore distribution during powder compact forming using an X-ray CT and mercury pore analyzer and experimentally investigated the how initial density slope affected powder compaction forming by employing the X-ray CT.

Hassani and Hinton [10] formulated an analytical solution of homogenization theory for various material models to be used in the finite element analysis. Also Takano *et al*. [11-12] presented a calculation of the elastic coefficient as a function of porosity and pore shape for compound materials and porous ceramic materials using homogenization theory.

In addition, as the relative density is one of the important factors in evaluating ceramic products, much effort to get high density products from the beginning of compact forming

*Corresponding author:
Tel : +02-2220-0436
Fax: +02-2298-6194
E-mail: ytkeum@hanyang.ac.kr

is in progress. Recently, researches on the optimum process parameters enabling high relative densities have been made. Roughly summarizing the researches on the parameter study of relative density, Jiang *et al.* [13-14] carried out experiments looking at the effect of the lubricant of a metal composite, the aspect ratio of the test material and the size of particles. Rendanz and Fleck [15] used a computer simulation technique to study the compaction of randomly distributed powders. Inter-particle friction and affined motion has been studied both for the compaction response and for the resulting yield surface. Procopio and Zavaliangos [16] simulated the multi-axial compaction for a granular media to study relative densities related to the particle shape and size as well as material properties. Consuelo and Lannutti [17] also examined the effect of particle size during the packing. Hassanqaur and Ghadiri [18] employed the distinct element method to simulate the bulk deformation, based on single particle properties. Briscoe and Rough [19] carried out an experiment to see the effect of friction between powder particles and the die.

Kim *et al.* [20] looked into the effects of repetitive pressure, repetitive velocity, and biased pressure on powder densification under repetitive compaction in room temperature. Also Shin *et al.* [21] presented the forming conditions to be able to improve the reproducibility by studying the changes in the forming density and sintering density in normal pressure sintering.

In this study, the arbitrarily-intensified powder compact is first modeled and the equivalent material property is introduced in the finite element analysis to simulate ceramic powder compaction. In addition, the optimal values of process parameters providing the maximum relative density are pursued on the basis of the response surface model obtained from the analysis of the experimental region of interest chosen by the full factorial design.

Forming Process Analysis

Modeling

Fig. 1 is a 2-dimensional view of the powder compaction device and ceramic powders before compaction. The ceramic powders are located inside the die and base punch stationary and are compacted to the desired shapes by the upper punch operating up and down. While the base punch and dies are stationary, the upper punch is movable so that repetitive loads can be applied to the powders.

Generally, homogeneous or non-homogeneous powders are modeled in the finite element analysis of a ceramic powder compaction process with the assumption that unit cells are periodically arrayed in hexahedron or cubic shapes. Although the powders are not periodically arrayed in a real compaction, the powders are modeled using a quasi-random multi-particle array, which can represent the non-periodicity and arbitrariness of the powder distribution by packing the particles one by one considering the powder array and the size distribution, position, and rearrangement of powder particles. After packing the particles to give contact between particle and particle or between tool and particles, the size and array of the particles are adjusted to make the desired relative density. In order to analyze green compacts whose initial relative densities are 0.554, 0.607 and 0.615, respectively, the size of an Al particle is fixed to 15 μm. Then Al_2O_3 particles whose sizes are 7.5 μm, 15 μm and 22.5 μm, respectively, are modeled. The models whose sizes of Al_2O_3 are 7.5 μm, 15 μm and 22.5 μm are called Model 1, Model 2 and Model 3, respectively.

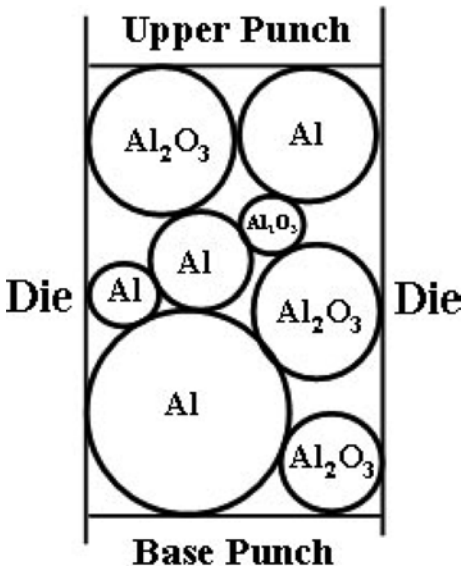

Fig. 1. 2-dimensional view of powder compaction device and ceramic powders.

In ceramic powder compaction forming, an important factor to control the relative density is the friction coefficient. Generally, the friction coefficient between the dry Al_2O_3 powders unlubricated is 0.35-0.50 and lubricated with zinc stearate is 0.7-1.0 [22]. To investigate the effect of various friction coefficients on the relative density of powder compaction, different friction coefficients between the powders are used in the analysis of the powder compaction forming process.

Formulation

The finite element formulation of stress fields, which is used to analyze the powder compaction forming process, is written as follows [23]:

$$\sum_{e=1}^{E}([K]\{u\}-\{F\})_e=0 \quad (1)$$

where [K] is the stiffness matrix obtained from the homogenized theory and [F] is the force vector. Homogenization theory is introduced to find the equivalent material property from the microscopic scale model for analyzing accurately macroscopic scale porous materials such as powder ceramics. For example, the homogenized elastic tensor, E^H_{ijkl}, is written as:

$$E^{H}_{ijkl} = \frac{1}{|Y|}\int_{Y} E_{jikl}\left(1 - \frac{\partial \chi^{kl}_{m}}{\partial y_{n}}\right) dY. \quad (2)$$

where E_{ijkl} is the elastic tensor and x^{kl}_{m} is the characteristic displacement. In the governing equation of a linear elastic problem, which is derived from the homogenization theory equations, the 2-dimensional powder compact Ω is assumed to be the assembly of micro-unit cells [23].

Forming Analysis

Analysis model and homogenized material property

In this study, the compound compact consisting of three aluminum and three alumina powder particles are modeled with 2-dimensional rods by using the quasi-random multi-particle array. A rod array model is often employed in numerical simulations because not only is there no big difference in the density, although it is less dense than a real powder compact, but also it clearly shows material behaviors and contact states [1].

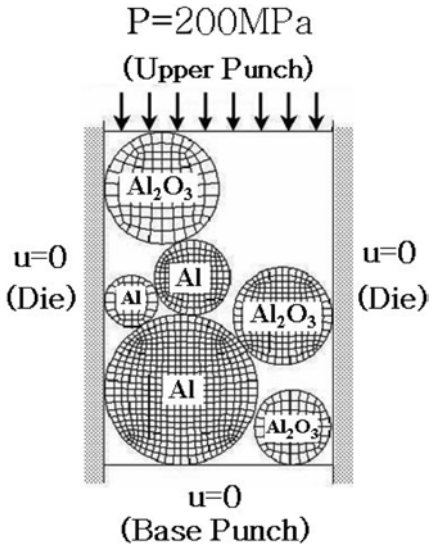

Fig. 2. Finite element modeling of ceramic powders and boundary conditions for simulating the powder compaction process.

For the elasto-plastic finite element analysis, powder particles are modeled with 4 node elements in a plane strain state, as seem in Fig. 2. Model 1 employs 526 nodes and 444 finite elements. Model 2 uses 695 nodes and 598 finite elements. Model 3 has 821 nodes and 714 finite elements. The upper punch, base punch, and die are modeled with mass elements.

The density, elastic modulus, Poisson's ratio and yield strength are the material properties used in the forming analysis. The homogenized elastic modulus is also employed. Table 1 shows the material properties of Al and Al_2O_3 used in the analysis. Fig. 2 presents the boundary conditions used in the finite element analysis. While the dies and base punch are assumed to be rigid, namely not deformable, the upper punch presses ceramic powders, taking 30 seconds up to the peak pressure P = 200 MPa.

For calculating the homogenized elastic modulus associated with porosities, the unit cell structure with a cross shaped porosity, which is similar to the porosity shape a of powder compact, is modeled with 2-dimensional finite elements (see Fig. 3). Then, the relative elastic modulus E_r is obtained using the homogenization method from the unit cell structures

Table 1. Material properties of Al and Al_2O_3

Material property	Al	Al_2O_3
Mass density (ρ)	$2.12(10)^3$ kg/m^3	$3.89(10)^3$ kg/m^3
Yield stress (YS)	28 MPa	300 MPa
Poisson's ratio (ν)	0.345	0.22
Elastic modulus (E)	62 GPa	375 GPa
Homogenized elastic modulus (E_h)	$E_r \times e^{-4.3387f}$ GPa	$E_r \times e^{-4.3387f}$ GPa

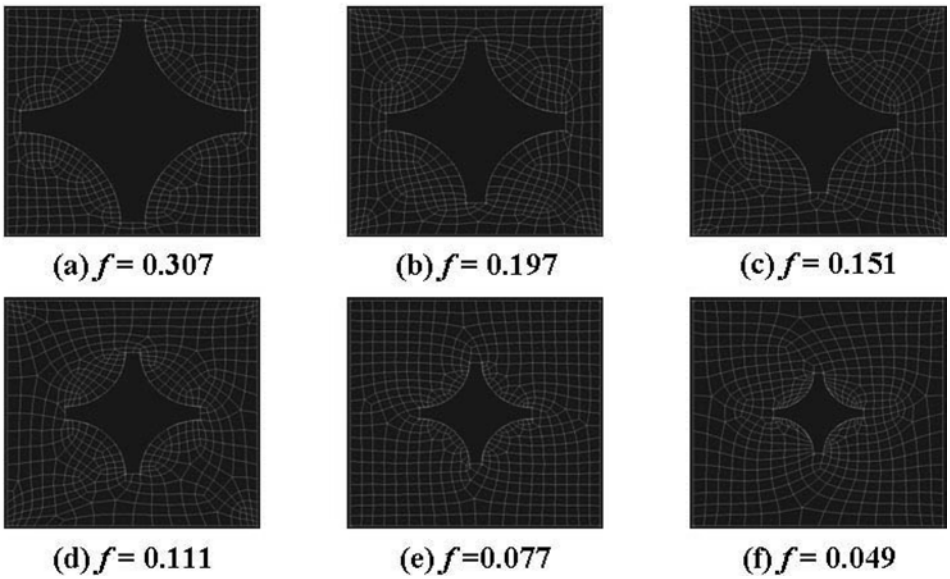

Fig. 3. Cross pore-solid models for calculating homogenized elastic modulus associated with porosities(f).

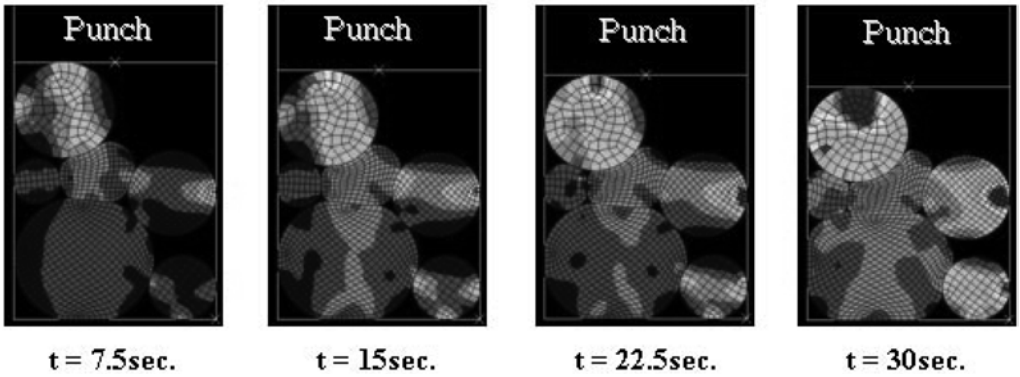

Fig. 4. Formed shapes and principal stresses of 6 particles during the powder compaction.

associated porosities f, and the homogenized elastic modulus E_h is calculated by interpolating E_r as follows:

$$E_h = E_r \times e^{-4.3387f}. \quad (3)$$

Numerical analysis

The powder compact forming process model is analyzed by employing the finite element method using both a micro-mechanics approach and a continuum-mechanics approach. In the micro-mechanics approach, the physical quantities such as stress and velocity can be different from those averaged in the macroscopic approach. In this method, the powder compact is regarded as an assembly of particles. Particles and gaps occupy the space inside the powder compact. Particles are defined as 1 and gap 0 in the density function. The simulation is performed using the elastic modulus E for 30 seconds taking up to the peak pressure P = 200 MPa. Fig. 4 shows the formed shapes of the 6 particles during the compaction. A micro-mechanics approach shows that the relative density gradually increases to 0.699, 0.730, 0.769, and 0.804 during the compaction.

In the continuum mechanics approach, the atomic structures of materials are neglected. All physical quantities are assumed to be represented with continuous mathematical functions. Therefore, stress and strain are defined at all points in the continuum. Using the homogenized elastic modulus associated with porosities E_h, as done in the micro-mechanics approach, the simulation is performed for 30 seconds. Relative densities are increased to 0.748, 0.778, 0.792, and finally to 0.816.

Fig. 5 shows a comparison of the relative density between FEM and the experiment done by Jiang *et al.* [2] The relative densities obtained by the continuum approach which introduces the homogenized elastic modulus associated with porosities in the analysis are closer to the experimental ones than those of the micro-mechanics approach. The reason for the sudden rise of relative density when the homogenized elastic modulus E_h is used in the continuum approach is why the E_h is small, which is calculated in the initially low relative density of the powder compact, namely the high porosity state, but E_h suddenly increases as the relative density increases.

Next, the analysis is performed under the condition

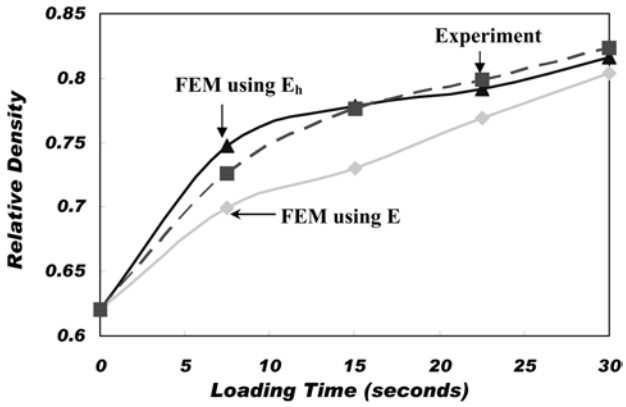

Fig. 5. Comparison of relative densities obtained from FEM analyses and experiment during the powder compaction.

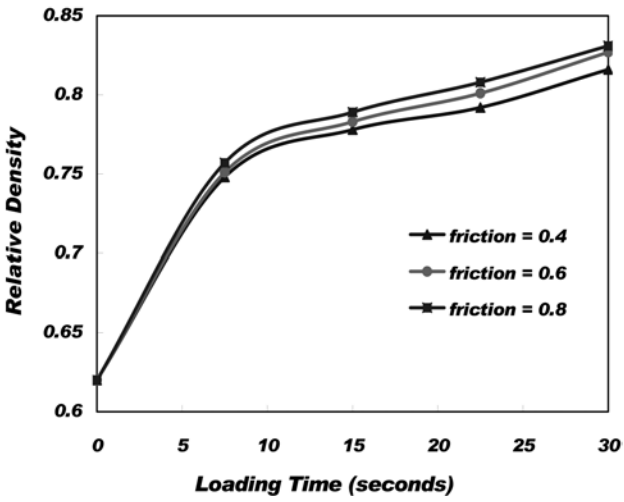

Fig. 6. Comparison of relative density among friction coefficients 0.4, 0.6, and 0.8.

where the friction coefficient between the powders is changed to 0.4, 0.6, and 0.8 while the friction coefficient between the powders and die is fixed. Fig. 6 shows the changes in relative densities with time as the friction coefficient changes. After 30 seconds reached to the peak pressure, the relative densities are 0.816, 0.827, and 0.831 when friction coefficients are 0.4, 0.6, and 0.8, respectively.

Process Parameters Optimization

Experimental region of interest

The optimization flow of process parameters of powder compaction followed in this study is seen in Fig. 7. After the experimental region of interest is set up by the full factorial design, the finite element analyses are performed for all cases in the region. The response surface called the "regression model," which is represented by the second order polynomial function of process parameters, is then found from the responses obtained from the analysis results. Finally, the optimal values of process parameters providing the maximum relative density are determined by the grid search method.

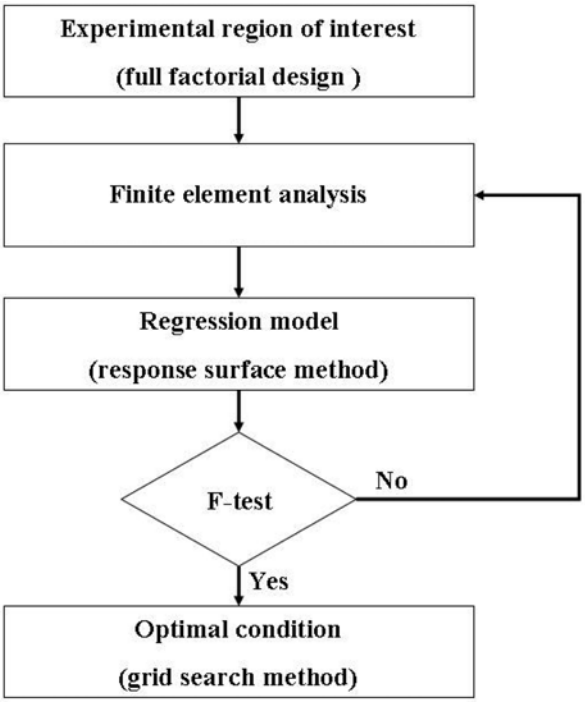

Fig. 7. Schematic flow for optimizing process parameters of powder compaction.

The Al_2O_3 particle size, amplitude of cyclic compaction, and friction coefficient are chosen as design variables and the experimental region of interest is set up by the full factorial design, as shown in Table 2. Next, the finite element analyses are performed a total of 27 times determined by the three variables and three levels. In every finite element analysis, the relative density and principal stress for 0, 1, 10, 100, and 1000 cycles of compaction pressure are calculated, as seen in Fig. 8, and the difference in relative density between 1 cycle and 1000 cycles is defined as the response.

Regression model

The response surface method, which was introduced by Box and Wilson [24], is to optimize approximately the variables after representing an analysis model with explicit functions. In this study, the response surface method is used for optimizing the powder compact process parameters defined in the previous section.

Approximately expressing the response surface obtained from the simulations done at the N experimental points selected by the experimental design with an objective

Table 2. Process parameters and levels for optimization

Process parameters		Levels		
		-1	0	1
Al_2O_3 particle size [μm]	x_1	7.5	15	22.5
Amplitude of cyclic compaction pressure[MPa]	x_2	125	100	75
Coefficient of friction	x_3	0.1	0.3	0.5

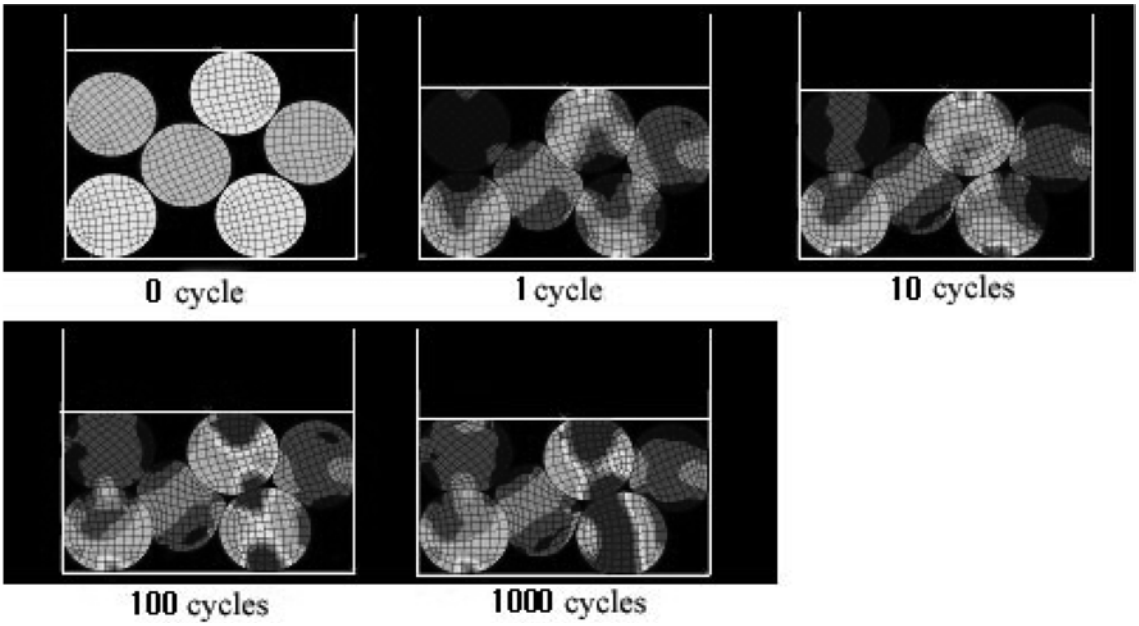

Fig. 8. Formed shapes and principal stresses associated with pressure cycles in the case of $x_1 = x_2 = x_3 = 0$.

function $\bar{y}$ as follows:

$$\bar{y} = X\beta + \varepsilon \quad (4)$$

Using the least square estimate about the response obtained from 27 simulations, the estimated regression model $\bar{y}$ can be expressed as follows:

$$\bar{y} = 0.218137 - 0.053844x_1 + 0.054244x_2 + 0.004089x_3 - 0.017792x_1x_2 - 0.000608x_1x_3 - 0.000608x_2x_3 + 0.038789x_1^2 + 0.000156x_2^2 - 0.003311x_3^2 \quad (5)$$

where x_1, x_2, and x_3 are the process parameters defined in Table 2.

The recurrence of the estimated regression model, which is evaluated through the F-test performed by variance analysis [25], is listed in Table 3. The regression model of Eq. (5) has a recurrence because of the rejection $F_{(0.05;9,17)} = 2.98$ when the level of significance is 5% and $F_0 = 204.43\ (10)^4$.

Optimal conditions

Eq. (5), which is derived as a result of the response surface method to optimize process parameters, can be graphically shown in Fig. 9, Fig. 10, and Fig. 11 when the remaining third process variable has a middle level. Fig. 9 shows that the variation of relative density increases with the Al_2O_3 particle size (−1 direction of x_1) and the amplitude of cyclic compaction pressure (1 direction of x_2) decreases. Fig. 10 shows that the variation of relative density when the friction coefficient becomes smaller (−1 direction of x_3) is not as big as much as that when the Al_2O_3 particle size is smaller (−1 direction of x_1). Fig. 11 implies that the increase in the variation of relative density when the amplitude of cyclic compaction pressure decreases (1 direction of x_2) is bigger than that when the coefficient of friction decreases (−1 direction of x_3). Therefore, the response surface model explains that the effects of the Al_2O_3 particle size and the amplitude of cyclic compaction pressure on the relative density is bigger than that of the friction coefficient in ceramic powder compaction forming.

In order to find the values of design parameters associated with the maximum relative density, the grid search method is used [26]. The optimal condition, in which the maximum relative density is 0.9390, is found when the Al_2O_3 particle size, the amplitude of cyclic compaction pressure and the friction coefficient are 22.5 μm, 75 MPa and 0.1103, respectively.

Table 3. Variance analysis of regression model

Degree of freedom of regression	9
Regression sum of squares	0.118352
Regression mean squares	0.01315
Degree of freedom of error	17
Error sum of squares	$1.09\ (10)^{-7}$
Mean square error	$6.43\ (10)^{-9}$
Total degree of freedom	26
Total sum of squares	0.118352
F_o = Regression mean squares / Mean square error	$204.43\ (10)^4$

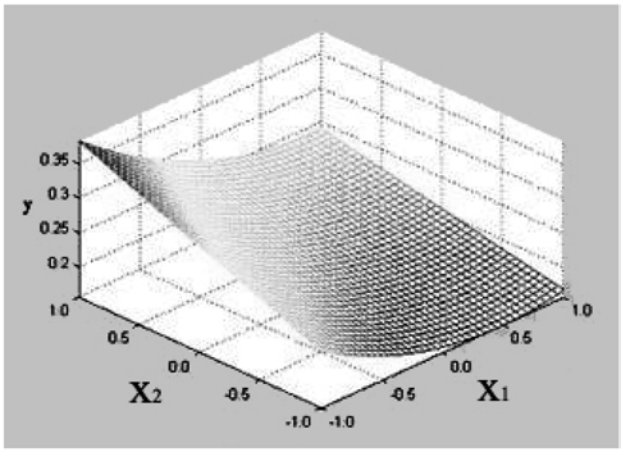

Fig. 9. Response surface model for Al_2O_3 particle size (x_1) and amplitude of cyclic compaction pressure (x_2) in the case of friction coefficient $x_3 = 0$.

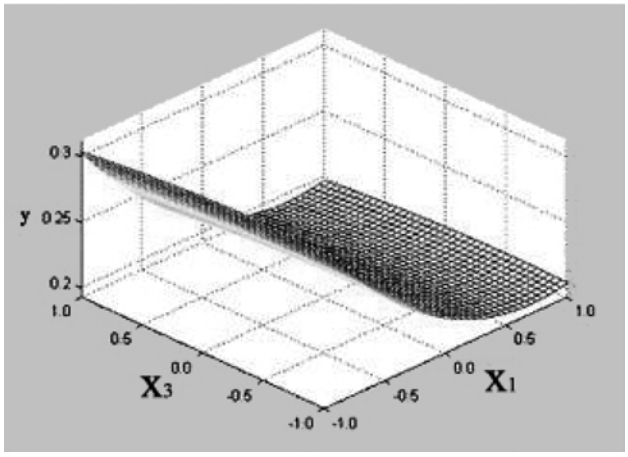

Fig. 10. Response surface model for Al_2O_3 particle size (x_1) and coefficient of friction (x_3) in the case of cyclic compaction pressure amplitude $x_2 = 0$.

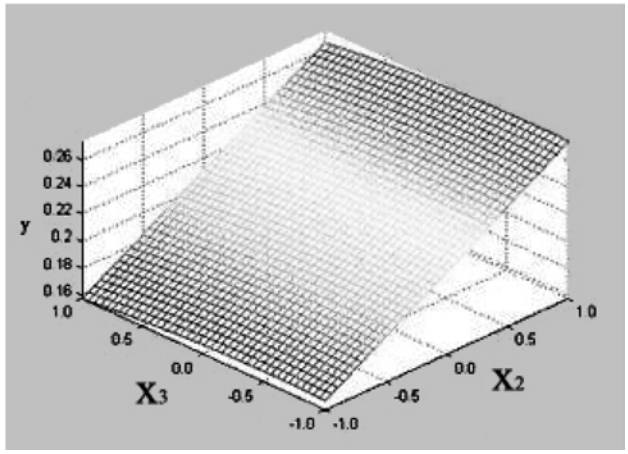

Fig. 11. Response surface model for amplitude of cyclic compaction pressure (x_2) and coefficient of friction (x_3) in the case of particle size $x_1 = 0$.

Conclusions

Multi-scale modeling and finite element analysis were performed to predict the relative density of ceramic powder compaction forming and the optimization of process parameters was carried out to maximize the relative density. Through the forming analysis and optimization, the following conclusions are made:

(1) The modeling of non-periodicity and arbitraries of ceramic powder particles can be successfully achieved by introducing a quasi-random multi-particle array.

(2) The ceramic powder compaction forming process can be accurately simulated by a multi-scale model and equivalent material properties obtained by employing the homogenization method.

(3) The relative density becomes bigger with the size of the Al_2O_3 particles, the amplitude of the cyclic compaction pressure, and coefficient of friction are smaller.

(4) The regression model enables to predict the relative density associated with compaction conditions and to provide the optimal conditions of process parameters related to the highest density of the green ceramic compact.

Acknowledgements

This work was supported by the research fund of Hanyang University (HY-2006-I). The authors appreciate Prof. R.H.Wagoner for discussions leading to these results.

References

1. W. Wu, G. Jiang, R.H. Wagoner and G.S. Daehn, Acta mater. 48 (2000) 4323-4330.
2. G. Jiang, W. Wu, G.S. Daehn and R.H. Wagoner, Acta mater. 48 (2000) 4331-4335.
3. X.J. Xin, P. Jayaraman, G. Jiang, R.H. Wagoner and G.S. Daehn, Metallurgical and Materials Transactions A, 33A (2002) 2649-2658.
4. N. Zahlan, D.T. Knight, A. Backhouse and G.A. Leiper, Powder Technology 114 (2001) 112-117.
5. H. Zipse, Journal of European Ceramic Society 17 (1997) 1707-1713.
6. T.A. Deis and J.J. Lannutti, Journal of the American Ceramic Society 81[5] (1998) 1237-1247.
7. P.K. Lu and J.J. Lannutti, Journal of the American Ceramic Society 83[3] (2000) 518-522.
8. P.K. Lu and J.J. Lannutti, Journal of the American Ceramic Society 83[10] (2000) 2536-2542.
9. P.K. Lu and J.J. Lannutti, Journal of the American Ceramic Society 83[6] (2000) 1393-1398.
10. B. Hassani and E. Hinton, Comput. Str. 69 (1998) 719-738.
11. N. Takano, Y. Uetsuji, Y. Kashiwagi and M. Zako, Model. Simul. Mater. Sci. Eng. 7 (1999) 207-231.
12. N. Takano, M. Zako and M. Ishizono, J. Comput.-Aided Mater. Design. 7 (2000) 111-132.
13. G. Jiang, G.S. Daehn, J.J. Lannutti, Y. Fu and R.H. Wagoner, Acta mater, 49 (2001) 1417-1441
14. G. Jiang, G.S. Daehn and R.H. Wagoner, Scripta mater, 44 (2001) 1117-1123.
15. P. Rendanz, N.A. Fleck, Acta Materialia, 49 (2001) 4325-4335.
16. A.T. Procopio and A. Zavaliangos, Mechanics and Physics of Solids, 53 (2005) 1523-1551.
17. M.K. Consuelo and J.J. Lannutti, Journal of the American Ceramic Society, 83[9] (2000) 2183-2188.
18. A. Hassanpour and M. Ghadiri, Powder Technology, 141 (2004) 251-261.
19. B.J. Briscoe and S.L Rough, Powder Technology, 99 (1998) 228-233.
20. K.T. Kim, G.S. Son and J. Suh, Journal of Korean Ceramic Society, 29[2] (1992) 136-142.
21. D.W. Shin, G.D. Kim, S.S. Park, C.S. Lim and S.W. Lee, Journal of Korean Association of Crystal Growth, 8[2] (1998) 356-364.
22. S. Turenne and P.E. Mongeon, Advances in Powder Metallurgy & Particulate Materials-1995 (1995) 155-164.
23. Y.T. Keum and J.W. Oh, Modelling and Simulation in Materials Science and Engineering, Institute of Physics Publishing, 13 (2005) 225-237.
24. G.E.P. Box and K.B. Wilson, Journal of the Royal Statistical Society, Series B., 13 (1951) p.1.
25. R.E. Wapole, R.H. Myers, S.L. Myers and k. Ye, in "Probability & Statistics for Engineers & Scientists 8th ed" (Pearson education, 2006).
26. Chen, D. Liu, X. Zhou, Y. Yang, X. Lu, L. Wang and X.J. Xin, Journal of Applied Polymer Science, 76[4] (2000) 481-487.