Simulation and Physical Experiment Study on Powder Metallurgy Preparation of Silicon Composite Powder

Qian Jia\textsuperscript{1, 2,*}, Zhaochong Ding\textsuperscript{1, 2}, Xiaona Zhang\textsuperscript{1, 2}, Xiaomeng Cao\textsuperscript{1, 2}, Haitao Teng\textsuperscript{1, 2} and Yongjun Li\textsuperscript{1, 2}

\textsuperscript{1}Grikin Advanced Materials Co. Ltd., Beijing, China
\textsuperscript{2}Beijing Technology Research Center for Sputtering Target Material Engineering of High Pure Metals, Beijing, China

*Corresponding author e-mail: jq@grikin.com

Abstract. The compaction and sintering processes of multi-component silicon powders, including single-action die compaction, uniaxial hot pressing and bidirectional hot compaction, were numerically performed by FEM (finite element method) modelling. The relationships of initial packing structure, compaction method, pressing pressure and sintering temperature between overall relative densities of multi-component silicon components were systematically discussed and studied. Meanwhile, various macro- and microscopic properties of silicon composite powders were carefully characterized, such as overall and local relative density, local stress distributions and void filling behaviour. The results show that fully compacted silicon composite targets with low internal stress can be obtained by using uniaxial hot pressing or bidirectional hot compaction method. And the physical experiments were carried out to verify the accuracy of the simulation results.

1. Introduction
Memory is an important part of integrated circuit semiconductor components, accounting for up to 20% of semiconductor products [1-5]. The most mainstream memory in the moment is DRAM, NAND Flash, NOR Flash, which accounts for about 95%. But the three major semiconductor memories themselves also have various shortcomings, such as the data of DRAM is volatile and it has small capacity; NAND Flash long delay; NOR Flash has a small capacity and a slow write and erases speed. Silicon alloy target is used in phase change memory chip manufacturing. Phase change memory has many advantages, such as low latency, read and write time balance, long life, low power consumption, high storage density and anti-irradiation, etc. However, there are still numerous in CM’s current research and development, such as that device power consumption and work speed are difficult to balance, thermal crosstalk problem at high density, the material needs to have both a high crystallization temperature and a low melting point, volume change before and after phase change affects device reliability. Many technical difficulties have not yet been completely overcome from materials and processes [6-9].

In this paper, the compaction and sintering processes of multi-component silicon powders, including single-action die compaction, uniaxial hot pressing and bidirectional hot compaction, were numerically performed by FEM (finite element method) modeling. The relationships of initial packing structure, compaction method, pressing pressure and sintering temperature between overall relative densities of
multi-component silicon components were systematically discussed and studied. Meanwhile, various macro- and microscopic properties of silicon composite powders were carefully characterized, such as overall and local relative density, local stress distributions and void filling behaviour. The results show that fully compacted silicon composite targets with low internal stress can be obtained by using uniaxial hot pressing or bidirectional hot compaction method. And the physical experiments were carried out to verify the accuracy of the simulation results.

2. Simulation method and conditions
FEM method was used to setup Single-action die compaction, uniaxial hot pressing and bidirectional hot compaction models of Si composite powders. In order to realistically simulate the whole PM process, the initial packing structures of multi-component powders with different particle sizes, which conform to a normal distribution, was firstly generated in DEM program. DEM, as a mature and effective dynamic simulation method, has been broadly applied in modeling the particle packing. Therefore, the governing equations and force models in DEM are not detailed and can be found in [10-14]. And then the initial packing densities of various heights were calculated by sectional area method. These data of initial packing densities were imported into FEM model as initial conditions, which was different with previous research. After that, other normal parameters were inputted, as well as materials property, boundary condition setting, contact definition, loading mode and temperature setting etc. Finally, subsequent compacting and sintering were simulated by using FEM method. The flowchart of the whole PM process is shown in Fig. 1(a).

The mesh division is shown in Fig. 1 (b), where each particle contains 5356 nodes and 4480 elements. Fig. 1 (c) gives the initial FEM model in the die before compaction. In the simulation, the die and punches are set to be rigid and Si composite powder is set to be elasto-plastic. The compaction is performed from the upper punch with the lower punch and the die being fixed.

Figure 1. (a) Flowchart in the numerical modeling on the PM process of Si composite powders; (b) mesh division for FEM model and (c) initial FEM model in the die before compaction.

In the simulation, the modified Shima-Oyane model [15, 16] is used to define the properties of multi-component Si alloy. In this model the flow yield stress is expressed as:
\[ F = \frac{1}{\gamma} \left( \frac{3}{2} \sigma^d \sigma^d + \frac{p^2}{\beta^2} \right)^{\frac{1}{2}} - \sigma_y \]  

(1)

Where \( \sigma_y \) is uniaxial yield stress, \( \sigma^d \) stands for deviatoric stress tensor, \( p \) represents hydrostatic pressure and \( \gamma, \beta \) are material parameters. \( \gamma \) and \( \beta \) can be expressed as:

\[
\gamma = (q_1 + q_2 \rho^{b_1})^{h_4}
\]

(2)

\[
\beta = (b_1 + b_2 \rho^{b_3})^{b_4}
\]

(3)

For multi-component Si alloy, \( q_1 = 0, q_2 = 1, q_3 = 3, q_4 = 1, b_1 = 6, b_2 = -6, b_3 = 1, b_4 = -0.5 \). Poisson’s ratio \( \nu \) and elastic modulus of multi-component Si alloy can be represented by:

\[
\nu = 0.5e^{-12.5(1-\rho)^2}
\]

(4)

\[
E = E_o \rho^{3.4}
\]

(5)

When defining contact, powders in the model are considered as deformable, while the die and punches are set as rigid bodies. The coefficient of friction between powders is set to be 0.2 using Coulomb friction model, while the contacts between the powders and the rigid bodies are considered as smooth. During compaction, the pressure from the upper punch will increase from 0 MPa to 150 MPa, and then it will be kept constant for a while and released. The temperature of hot pressing is 600 °C.

3. Results and discussion

3.1. Initial packing density

Fig. 2 (a) gives stable static initial packing structure with different particle sizes by DEM. It can be seen that large pores exist on the die boundary, which caused by the boundary effect of die wall.

![Figure 2](image.png)

Figure 2. (a) Initial packing structures with different particle sizes by DEM; (b) evolution of relative density of initial packing structure with height, where the inset figure shows the local results presented by red dotted lines.

Meanwhile, Fig. 2 (b) shows that the evolution of relative density of initial packing structure with height, where the inset figure shows the local results presented by red dotted lines. It can be found that stratification generates in the distribution of initial packing density, which consistent with Fig. 2 (a), the initial packing density of bottom and end faces is the lowest. In addition, one more case can be seen in
Fig. 2 (b) that the initial packing density of middle part fluctuates with increasing height, which shows that this part is an irregular stacked structure.

3.2. Macro characteristics
Relative density-pressure relationship for Si composite powder mass using different pressing methods was shown in Fig. 3 (a), where the inset figures indicate the distribution of relative density at 150 MPa. As shown in Fig. 3 (a), with the increase of pressure, the initial relative density increase, and the packing structure becomes denser. However, high relative density component can be obtained with hot pressing comparing die compaction at same compaction pressure. This phenomenon can be explained by material softening. Temperature can decrease yield strength of Si Alloys, so high relative density can be obtained at low compaction pressure using hot pressing method. At the same time, we can see that the relative density distribution of hot pressing is more uniform, indicating that hot pressing can gain more uniform and denser green target.

Meanwhile, internal stress distribution is studied. Here, the equivalent von Mises stress is given by [17, 18]:

\[
\bar{\sigma} = \left( (\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2 \right)^{1/2} / \sqrt{2}
\]  

(6)

Where \(\sigma_1, \sigma_2, \sigma_3\) are the principal Cauchy stresses along three main axes. Fig. 3 (b) gives the equivalent von Mises stress of different compaction methods as a function of pressure during compaction. From this figure, it can be found that lower stress can be obtained in hot pressing, so high quality green target is easily gained by using hot pressing.

**Figure 3.** (a) Relative density-pressure relationship for Si composite powder mass using different pressing methods, where the inset figures indicate the distribution of relative density at 150 MPa; (b) equivalent von Mises stress of different compaction methods as a function of pressure during compaction.

3.3. Micro characteristics
Axial flow and radial flow of Si composite powders are studied in this part. Fig. 4 (a) shows the evolution of axial displacement with relative height during compaction using different compaction methods, where the inset figures represent overall particulate flow. It can be found that hot-pressed axial flow is slower and smaller than single-action die compaction flow. Meanwhile, Fig. 4 (b) gives the evolution of radial displacement with radial distance during single-action die compaction. From Fig. 4 (b), it can be seen that the particles in the upper part of the molding flow toward the center, and the particles in the lower part flow to both sides. The flow in the middle part is the most intense.
Figure 4. (a) Evolution of axial displacement with relative height during compaction using different compaction methods, where the inset figures represent overall particulate flow; (b) evolution of radical displacement with radical distance during single-action die compaction.

3.4. Physical experiment
Fig. 5 gives the morphology of Si alloy target prepared by bidirection hot pressing. As shown in Fig. 5, complete crack-free Si alloy target has been produced by bidirection hot pressing, indicating our simulations are robust and reliable.

Figure 5. The morphology of Si alloy target prepared by bidirectional hot pressing

4. Conclusion
Cold uniaxial die compaction, single-action hot pressing and bidirection hot pressing of Si composite powders were numerically reproduced by using FEM method. The impacts of initial packing structure, compaction method, pressing pressure and sintering temperature on overall relative densities of multi-component silicon components were studied. Following conclusions can be drawn: (1) High relative density and low internal stress can be obtained at low compaction pressure using hot pressing method. (2) Hot-pressed axial flow is slower and smaller than single-action die compaction flow.

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