Journal of Alloys and Compounds 741 (2018) 473–481

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

MPFEM simulation of compaction densification behavior of Fe-Al composite powders with different size ratios

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ARTICLE INFO

Article history:
Received 19 October 2017
Received in revised form
3 January 2018
Accepted 14 January 2018

Keywords:
MPFEM simulation
Fe-Al composite powders
Compaction
Densification mechanism
Powder metallurgy

ABSTRACT

In this paper, 2D single-action die compaction process of Fe-Al composite powders with different size ratios was simulated via the multi-particle finite element method (MPFEM) from particulate scale. Different initial packing structures generated by discrete element method (DEM) were imported into FEM model (where each particle was discretized for mesh division) for compaction. The compaction process was reproduced and the densification dynamics and mechanisms were analyzed and identified based on the evolution of macro and micro properties of the compact. The results indicate that, when the Al contents in the composite powder and the compaction pressure are fixed, higher relative densities can be obtained at smaller Fe/Al size ratios. During compaction, large stresses are mainly concentrated within those contacted Fe particles (near the surface region), forming the contact force network which impedes the compaction densification. Upon unloading, the contact force network is broken, and most internal stresses are released while only small amount of residual stresses are remained within Fe particles, which is susceptible to cracking or even failure during further processing. The smaller the Fe/Al size ratio is, the more complete is the release of the residual stress. During compaction, large voids (or pores) formed in the initial packing are filled by particle rearrangement (especially the rearrangement of small Fe particles) and plastic deformation of Al particles. However, there are still some small enclosed pores left in the final compact, which will lead to non-uniform deformation of adjacent particles and stress concentration during the subsequent sintering process.

1. Introduction

Compared with the conventional solid materials, porous materials are fascinating due to their unique advantages such as low volume density, high specific strength and specific surface area, light weight, effective sound and heat insulation, and good permeability etc. Among a variety of porous materials, metallic porous materials are widely used in many industrial fields because of their high mechanical strength and thermal shock resistance, satisfactory machinability and weldability etc. [1]. But they also indicate insufficient strength at elevated temperature, relatively weak anti-oxidization and anti-corrosion properties, which limited their further application in corresponding area. Normally, these disadvantages in properties can be compensated by Fe_3Al or FeAl matrix intermetallics which have not only superior anti-oxidization and anti-corrosion properties, excellent specific strength and mid-temperature strength, but also low price of raw materials. Under this circumstance, fabricating Fe-Al intermetallic porous materials can efficiently improve their high temperature anti-oxidization and anti-corrosion properties, so that they can work in severe environment for high temperature gas dedusting and liquid filtration etc. [2–6]. Therefore, in the past decades, much work was carried out in this regard to fabricate Fe-Al intermetallic porous materials. Based on the intense Kirkendall effect induced by the significant difference of diffusion coefficient between Fe and Al elements, Gao et al. [7–9] used die compaction plus reaction sintering to produce Fe-Al intermetallic porous material, but these studies were mainly focusing on the reaction sintering stage. In comparison, the compaction stage is also of key importance in powder metallurgy (PM) production, but corresponding studies are less carried out. Actually, a high performance compact with high relative density, uniform density and stress distributions is the precondition for the production of PM component with superior properties. Therefore, in recent years, some researchers have forwarded their research interests to the compaction of Fe-Al composite powders.

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https://doi.org/10.1016/j.jallcom.2018.01.198
0925-8388/

Physically, several experiments were conducted to identify the relationship between the relative density of the compact and the pressure during compaction. However, physical experiments are unable to quantitatively characterize the local density distribution, stress distribution, and particle flow behavior in situ, especially the nonlinearity features in geometry, materials, and contact during compaction all increase the difficulties of physical experiments [10–14]. With the advent of various yield criteria of powder materials proposed by Kuhn, Green, Shima, Gurson, Doraivelu etc. [15–19], Drucker-Prager-Cap model [20] and Cam-Clay model [21], the powder compaction process was further understood. These models were successfully used in FEM modeling to characterize powder flow behavior during compaction. Under this background, a traditional macro continuous FEM simulation method, in which the powder mass is regarded as a continuum with uniform void distribution, was proposed to solve the problems arising from physical experiments. In addition to the relationship between overall relative density and compaction pressure, this method can also analyze local relative density and distribution, stress distribution, and powder displacement in the compact upon compaction from macro continuous scale. Therefore, as reported in our previous work, the single-action die compaction of pure metal powders [22–24] and composite powders [25,26] has been systematically investigated by this method. Even though the traditional FEM can to some extent solve the problems in physical experiments, it is really hard to deal with the important issues like dynamics and contact mechanics from particulate scale based on the aforementioned continuum assumptions. However, this deficiency can be overcome by molecular dynamics based DEM (discrete element method) simulation. DEM has been widely applied to generate various packing structures of spherical and non-spherical particles [27–30], but its effectiveness in modeling the compaction of powders is restricted to limited relative density (e.g. $\rho < 0.85$) [31]. For larger relative density and extra plastic deformation in PM compaction, a new method MPFEM (multi-particle FEM) has been developed and successfully applied in modeling powder compaction [32–47], but less work was conducted on the compaction of Fe-Al composite powders from particulate scale. One good example of the MPFEM was reported by Wu et al. who simulated 2D compaction process of Fe-Al composite powders by this method, but only the compaction of ordered initial packing structure was considered [44]. Actually, most powders before compaction are in random other than ordered packing states. In our previous work, the compaction of Fe-Al composite powders with random initial packing structures was modelled by MPFEM. But the research was mainly focusing on the Fe and Al powders with equal particle size [48], further systematic and intensive studies on the compaction of Fe-Al composite powders with different particle sizes are needed.

In this paper, single-action die compaction of binary Fe-Al composite powders with different particle size ratios was numerically simulated using MPFEM from particulate scale. Various initial packing structures before compaction were generated by DEM modeling and then imported into FEM model for compaction. The effects of particle size ratio on the relative density and distribution, stress and distribution, particle morphology evolution, pore filling and stress/force transmission upon compaction and unloading were systematically studied, and corresponding densification mechanism was analyzed.

2. Simulation method and conditions

2.1. Model setup

The particulate scale numerical simulation was carried out using commercial MSC.Marc software. To reduce the assumptions and more realistically reflect the actual process, DEM dynamic modeling was utilized to generate the initial random binary packing structure which was then imported into the FEM model for compaction. Fig. 1 (a) shows the structures of the obtained binary random initial packings before compaction, where small and large disks represent Fe and Al particles, respectively. With the content of Al particles being fixed at $X_{Al} = 25$ wt%, different size ratios of small Fe and large Al particles (e.g. $R_{Fe}/R_{Al} = 1{:}2, 1{:}3, 1{:}4, 1{:}5$) are chosen for compaction. It is worth to mention that the selected composition for study is also concerned by other researchers [5,6,8,9]. The mesh division of each particle is shown in Fig. 1 (b), which contains 132 elements and 169 nodes. At the interface of two contacted particles, the Coulomb friction model was used and expressed as:

$$\sigma_{fr} = -\mu\sigma_n \frac{2}{\pi}\arctan\left(\frac{v_r}{r_{v_{cnst}}}\right)t \tag{1}$$

where σ_{fr} is the tangential (friction) stress; σ_n is the normal stress; μ is the friction coefficient; t is the tangential vector in the direction of the relative velocity; v_r represents the relative sliding. Physically, the value of $r_{v_{cnst}}$ can be seen as the value of the relative velocity below which sticking occurs.

In the simulation, the yield stress can be expressed by:

$$\sigma_y = C(\varepsilon_0 + \bar{\varepsilon})^n + D\left(\dot{\bar{\varepsilon}}\right)^k \tag{2}$$

where ε_0 is initial yield strain; $\bar{\varepsilon}$ is equivalent strain; $\dot{\bar{\varepsilon}}$ is equivalent strain rate; parameters C, D, n and k are material constants. Initially, the equivalent strain and equivalent strain rate were assumed to be zero so that the initial yield strain can be calculated by material constants C and n, and Young's modulus (Y) in von Mises material model. The von Mises stress is given by:

$$\bar{\sigma} = \left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]^{1/2} \Big/ \sqrt{2} \tag{3}$$

where σ_1, σ_2, and σ_3 are the principal Cauchy stresses along three main axes. The equivalent strain rate is:

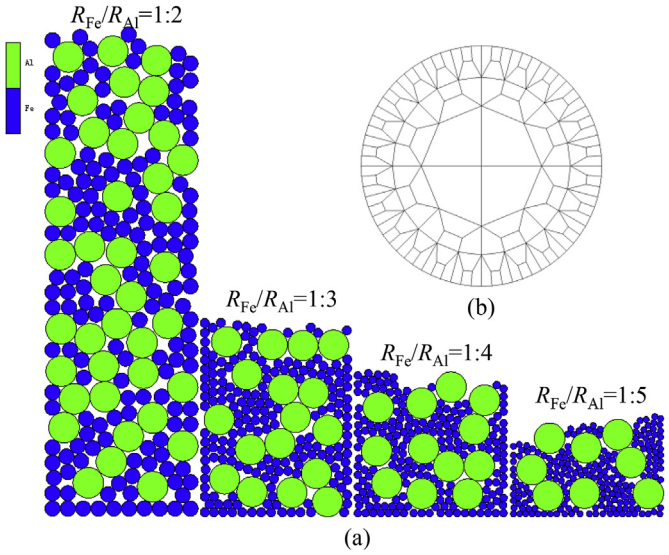

Fig. 1. DEM generation of initial binary random packing structures with different Fe/Al size ratios (a) and mesh division for an individual particle (b).