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Viscoelastic discrete element model of powder sintering

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ABSTRACT

This paper presents an original viscoelastic model of powder sintering developed within the discrete element framework. The viscous model used by other authors has been enriched by adding a spring connected in series to the viscous rheological element. In this way elastic and viscous effects in the particle interaction during sintering are treated using the Maxwell viscoelasticity. The new numerical model has been verified through simulation of simple problems of free sintering and sintering under pressure. Sintering processes have been treated as isothermic. In order to accelerate the analysis an algorithmic mass scaling has been used allowing to use larger time steps in the explicit time integration scheme. The results obtained using the new model are consistent with the standard viscous model. At the same time, a much better efficiency of the new model in comparison to the standard viscous one has been found because the critical time steps required by the viscoelastic model are much larger than those required by the viscous model. The new model has been applied to the simulation of real process of sintering of NiAl powder. The kinetics of sintering indicated by the evolution of density has been studied. The comparison of numerical and experimental results has shown a good performance of the developed numerical model.

1. Introduction

Sintering is a manufacturing process used for making various parts from metal or ceramic powder mixtures. Sintering consists in consolidation of loose or weakly bonded powders at elevated temperatures, close to the melting temperature with or without additional pressure. Changes of the microstructure during sintering have been shown in Fig. 1. In the initial stage (Fig. 1a) cohesive bonds are formed between particles. When the sintering process is continued, the necks between particles grow due to mass transport (Fig. 1b). Surface and grain boundary diffusion are normally dominant mechanisms of mass transport in a sintering. The main driving force of sintering is reduction of the total surface energy of the system. As a result of the stresses in the neck and the surface tension the particles are attracted to each other, which leads to the shrinkage of the system. The described processes – shrinkage and mass transport – lead to the reduction of material porosity. Sintering is a complex process influenced by many factors including technological ones such as temperature, sintering time, pressure and atmosphere which determine the properties of sintered materials [9,32,65,8].

Modelling can be used to optimize and to understand the sintering process better and improve the quality of sintered components. Modelling of the sintering process is one of the most challenging problems in material modelling. There are different approaches in modelling of sintering processes, ranging from continuum phenomenological models to micromechanical and atomistic ones. Different sintering models have been reviewed in [44,49,16,20]. In the continuum approach, the porous powder under compaction is treated as a continuous medium at the macro-scale. Its deformation behavior is described by constitutive equations based on modified theory of solids. Constitutive equations of continuous media belong to the class of phenomenological models in which model parameters are obtained by fitting experimental data. Well-known phenomenological sintering models are those developed by Abouaf et al. [1], Duva and Crow [13], Cocks [11], Sofronis and McMeeking [58], and Ponte [7]. Phenomenological approaches have been summarized by Olevsky [45], Exner and Kraft [16], Cocks [12] and German [21,23].

Phenomenological theories do not take into consideration the microstructure of the material. Microstructural changes during sintering are taken into account in micromechanical models. A number of micromechanical models of sintering are based on a particle representation of porous powder material undergoing the sintering process. In particle models, the interaction of particles and the local problems of particle necks are considered. Sintering is treated as a collective result of thermally activated adhesion processes which result in the growth of contacts between particles. Sintering models at the particle scale have been used in the classical works on sintering. Frenkel [17] and Kuczynski [37] studied mechanisms of neck growth and shrinkage for the early sintering stages (particle bonding) using a two-sphere model. The two-particle model has been extrapolated for

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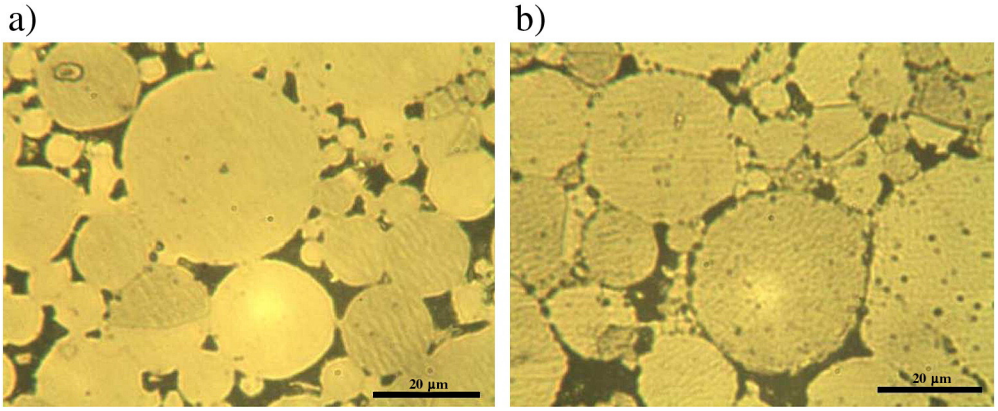

Fig. 1. Microstructure evolution during sintering of NiAl: a) early stage, b) final stage.

the intermediate shrinkage state by Kingery and Berg [35]. Coble [10] developed a cylindrical pore model, a spherical pore model for the late sintering stages was developed by MacKenzie and Shuttleworth [43]. More sophisticated models taking into account the superposition of various sintering mechanisms have been developed by Ashby [4], Arzt [3], and Exner and Arzt [15].

Growing capabilities of computational techniques increased the possibilities to employ particle sintering models. Sintering models have been implemented within the discrete element method which allows us to model interaction of large collections of particles [50,42,41,46,31,25,26,66]. Parhami and McMeeking [50] have implemented the particle sintering model derived by Coble [10] in the quasi-static formulation of the lattice type discrete element method to study free and pressure-assisted sintering. The concepts of Parhami and McMeeking have been incorporated in the dynamic formulation of the discrete element method by Martin et al. [42] and used for investigation of free sintering of metallic powders. A similar model has been applied by Henrich et al. [26] to simulate the free and pressure-assisted solid-state sintering of powders with special attention to the grain rearrangement during sintering. The effect of particle size distributions on sintering has been studied by Wonisch et al. [66]. The two-particle models of sintering implemented within the discrete element method [50,42,66] can represent properly the microstructure of a sintered material at early and intermediate stages of sintering. We can extend its use very carefully to higher densities, but we must remember that for compact solids these models lose their physical background, that is, they no longer represent a microstructure and can be treated as a mere way of discretization [60]. An interesting extension of the particle model for the final stage of sintering has been presented in [31], where the transformation of the particle model to a polyhedral one at a certain level of the process was proposed.

The macroscopic behavior of sintered materials is a result of a complex combination of elastic, viscous, plastic and thermal deformation depending on the processes occurring at the microscopic and atomistic levels [67,6]. Different deformation mechanisms dominate at different stages of a powder metallurgy process [2]. Although deformation during sintering itself is governed mainly by the viscosity, the material does maintain certain elasticity [39,38]. Phenomenological sintering models generally incorporate mechanisms of thermal and elastic deformation along with the viscous creep flow [19,67,30,34] although there is little knowledge of elastic properties during sintering. Experimental data on elastic properties at high temperatures in most cases do not cover the temperature ranges of sintering [40]. Due to insufficient data, elastic deformation in sintering models in most cases has been simply approximated in constitutive models of sintering [22,23]. Accounting for elastic effects may be important for a proper evaluation of stresses and reversible strains during sintering [34]. Experimental measurements such as those presented in [39,38] show important changes in the value of the Young's modulus during sintering and allow us to hope that future experimental investigation will enable a better understanding of elastic effects during sintering.

In the discrete element models of powder metallurgy process cited above, cf. [50,26,66,46], the sintering stage has been modelled assuming the viscous flow and neglecting elastic behavior. This paper presents a consistent viscoelastic model of particle interaction which allows us to keep elastic and viscous components of deformation. Accounting for elastic effects may influence the distribution of forces in the heterogeneous particulate material and have some importance to the evaluation of stresses during sintering and subsequent cooling.

The new sintering model has been implemented in the authors' own discrete element code [53,56,48,55,54]. The numerical model is verified by simple tests of two particle sintering as well as by more realistic tests of sintering of a cylindrical specimen composed of several hundred particles. The performance of the new viscoelastic model has been compared with that of the standard viscous model. While general agreement in the results has been observed, it has been found that the new model offers a much better numerical efficiency since it enables the use of a much larger time step in an explicit time integration of equations of motion. This is an important advantage of the newly developed model.

2. Numerical model of sintering

Numerical model of sintering is developed within the framework of the discrete element method which assumes that a particulate material can be represented as a collection of spherical particles interacting with one another. Following Martin et al. [42] the rotational motion of the particles and tangential interaction has been neglected in the present formulation. This should be favorable for particle rearrangements. Nevertheless, further development of the model should include tangential forces as well as the moment interaction between particles.

2.1. Discrete element formulation

The translational motion of rigid particles is described by means of the Newton's equations of rigid body dynamics. For the i-th element we have

$$m_i \mathbf{u}_i = \mathbf{F}_i, \tag{1}$$

where $\mathbf{u}_i$ is the element centroid displacement in a fixed (inertial) coordinate frame, $\mathbf{m}_i$ — element (particle) mass, and $\mathbf{F}_i$ — the resultant force being the sum of all the forces applied to the i-th element due