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Sintering Multi-scale Virtual Reality

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Abstract

The directions of further developments in the modeling of sintering are pointed out, including multi-scale modeling of sintering, on-line sintering damage criteria, particle agglomeration, sintering with phase transformations. A true multi-scale approach is applied for the development of a new meso-macro methodology for modeling of sintering. The developed macroscopic level computational framework envelopes the mesoscopic simulators. No closed forms of constitutive relationships are assumed for the parameters of the material. The model framework is able to predict the final dimensions of the sintered specimen on a global scale and identify the granular structure in any localized area for prediction of the material properties.

Keywords : sintering, multi-scale modeling, monte-carlo method, finite-element method

1. Introduction

As regards the current theory of sintering, one can distinguish the instigation period (1940s-1950s), and the "golden age" of progression and discovery (1950s-1970s).

In the mid 1980s practical demands necessitated the creation of a new approach connected with the use of continuum mechanics, which has been successfully applied to the description of macroscopic behavior of powder materials during sintering. This approach formed a scientific direction, which can be designated as a continuum theory of sintering [1-5]. Despite its successful implementation for the prediction of shape distortions and density distributions in sintered bodies, a number of serious problems remain to be solved.

In particular, existing theories require a link between the meso- and macroscopic descriptions of sintering, the necessity of the development of corresponding multi-scale approaches in the constitutive modeling of sintering should be noted.

2. Meso-Scale Simulation of Sintering

Sintering theory was traditionally developed either as the application of complex diffusion or viscous flow mechanisms to a simple geometry or as complex evolution of microstructure with simple diffusion mechanisms. A model needed to be elaborated that can treat in detail both the evolution of a realistic mesostructure and the sintering mechanisms of a realistic powder compact. For this purpose (see Fig. 1), the stereological theory of sintering has been incorporated in a lattice-based, Monte Carlo model, also known as the Potts model [6], which allowed tracking microstructural changes in a complex and realistic geometry.

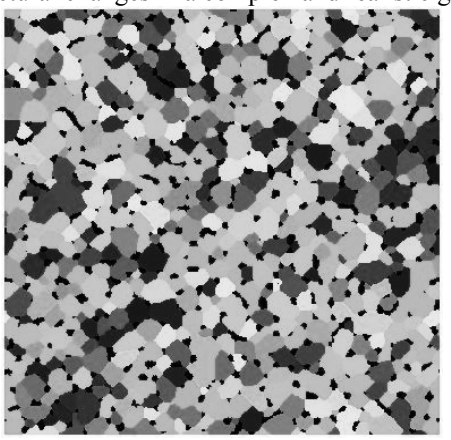

Fig. 1 Microstructure Colored features are grains, black features are pores

A first attempt of the development of a multi-scale theory of sintering, including both the meso-scale and macroscopic continuum mechanics – based sintering models, has been undertaken [6].

3. Multi-Scale Computational Approach

While the previous multi-scale approach [6] assumed the direct usage of the mesoscopic data for the one-time determination of the macroscopic constitutive parameters, the developed computational research framework enables engineering system-level analyses without the need to derive

macroscopic, averaged constitutive equations for irreversible processes. In order to predict the evolution of macroscopic stresses and temperatures in a component, macroscopic finite elements are used. Every element of the macroscopic mesh contains internal meso-scale meshes. The macroscopic accumulated irreversible strains in the macroscopic elements are determined as the volume average of the mesoscopic strains. Accumulation of the macroscopic strains is accompanied by the development of the macroscopic elastic stresses that maintain compatibility between different elements. In order to find these stresses, the tensors of macroscopic elastic constants are estimated for every macroscopic finite element. The method of homogenization is based on elastic energy considerations [7]. Elastic constants appear as derivatives of the elastic energy with respect to macroscopic elastic strains. If the average material constants are found, the solutions of macroscopic FEM problems give the volume distribution of macroscopic stresses and temperatures that are used as boundary conditions at the mesoscopic scale.

The original approach, described above, is at the stage of preliminary testing. It should enable, for the first time, the determination of the constitutive equations for sintering based upon virtual experiments, thereby avoiding costly physical tests. The existing governing equations for sintering will be verified and further developed.

4. Multi-Scale Modeling of Sintering with Inclusion

As an important example for the modeling, sintering with an inclusion has been considered (Fig. 2). Besides the predictions of the evolution of the macroscopic shape and porosity evolution, which are common in the continuum modeling of sintering processes, this case study includes the analysis of each finite element as a representative domain with evolving pore-grain structure. Fig. 2 demonstrates two finite elements' instantaneous meso-structures, corresponding to the inclusion and surrounding matrix, respectively. Currently, a comprehensive parallel processing algorithm enabling the analysis of more complex cases with substantially larger number of finite elements is being developed.

5. Summary

A multi-scale approach for modeling sintering processes has been developed. Macroscopic shape distortions, porosity spatial distribution, and local pore-grain structure can be analyzed simultaneously based on the elaborated model framework. The modeling schematics do not require an explicit form of macroscopic constitutive equations. An example of multi-scale modeling of sintering with inclusion is considered. The development of a parallelization algorithm enabling the consideration of more complex cases involving substantial numbers of finite elements is currently under development.

6. Acknowledgements

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