Towards a more realistic discrete element model of solid-state sintering: grain growth and non-spherical particles

Brayan PAREDES GOYES

Supervisors: Christophe MARTIN and David JAUFFRES

Friday, December 2nd 2022 – 2:00 p.m.

Amphi Wilfrid Kilian (ISTerre, Domaine Universitaire)

Jury :

- Marc BERNACKI, Professeur, Mines ParisTech (Rapporteur)
- Guillaume BERNARD-GRANGER, Directeur de Recherche, CEA Marcoule (Rapporteur)
- Rajendra BORDIA, Professeur, Clemson University (Rapporteur)
- Helen REVERON, Directrice de Recherche CNRS, MATEIS (Examinatrice)
- Jérôme DURIEZ, Charge de Recherche INRAe, RECOVER (Examinateur)
- Bruno CHAREYRE, Maître de conférences, UGA (Examinateur)

Abstract: Solid state sintering is a widely used powder processing technique for ceramics and metals. The treatment is carried out at high temperatures, below the melting point. Consolidation, densification, and grain growth occur during sintering. The discrete element method (DEM) has been effectively applied for modeling densification and consolidation at the mesoscale for spherical particles. Nevertheless, grain growth affects sintering during the intermediate and final stages. It is not considered by actual DEM simulations. Here, a realistic grain growth model is developed. The mechanisms considered are surface diffusion and grain boundary migration. The standard densification model, based on grain boundary diffusion and surface diffusion, is refined to take into account large particle size ratios. Both models are coupled for studying the microstructural evolution during sintering until the relative density approaches 0.90. The densification and grain growth kinetics, the sintering trajectories, and the evolution of the particle size distribution are analyzed for an initial packing with realistic size distribution. The results are in good agreement with grain growth experimental data from the literature for conventional sintering of alumina. Grain growth is particularly problematic and difficult to avoid for nano-powders. A possible approach to mitigate grain growth is two-step sintering, which uses a combination of high and low temperatures during the sintering thermal cycle. DEM simulations are employed to explore the mechanisms that can explain the success of two-step sintering. Another means to improve the realism of DEM sintering models is to consider actual particle shapes instead of spheres. This is particularly relevant for sintering since the driving force is the local curvature. The real shape of particles can be captured using the level set discrete element method (LS-DEM). An optimization-based contact detection algorithm is proposed to reduce computational cost. The proposed LS-DEM implementation is a proof of concept of its potential effectiveness for sintering. For illustration, simulations of ellipsoidal particle packings with elastic and

sintering interactions are shown. Sintering simulations allow to analyze the influence of the particle aspect ratio on shrinkage.
Keywords: sintering, discrete element method, grain growth, nano-powders, two-step sintering, non-spherical particles, Level-Sets