Discrete element model for coupled thermal and electrical phenomena in spark plasma sintering

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1. Introduction

The increasing interest in Spark Plasma Sintering (SPS) stems from its potential as a sustainable and ecological powder consolidation process. In this process, the powder is simultaneously subjected to mechanical pressure and heated by Joule heating, generated as an electrical current flows through the powder and tools. Initially, the powder consists of loosely bonded particles. As the process progresses, the particles become connected through necks, which grow over time due to diffusion and mass transport. SPS process involves complex interdependence of electrical, thermal, and mechanical phenomena. Therefore, to develop a comprehensive model for the SPS process, a coupling approach is required where all these phenomena are integrated together. Discrete Element Method (DEM) is a suitable choice as it allows microscopic modelling of the sintering process. In DEM based approach, each particle in the powder is treated as a discrete element, allowing precise representation of microscopic structures and interactions. In this work effective thermal and electrical conductivity of metallic powders undergoing densification is studied and a coupled thermo-electric DEM model is developed. The simulation results are validated using our own experimental measurements.

2. Experimental work

NiAl powder with spherical morphology (as shown in Figure 1a) was sintered under different pressures and temperatures to obtain four samples with varying density levels. Heating rate of 100K/min was used during all the processes. Microstructural analysis using SEM showed the sintering mechanism, beginning with neck formation in the low-density samples, followed by neck growth as the density increased, and ultimately resulting in a fully densified microstructure at higher densities. Figure 1b illustrates SEM image of the fractured surface showing necks and texture in the grain boundaries. This observation is important for incorporating grain boundary resistance in the

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model. Thermal and electrical conductivities was measured for all the samples, showing increase in conductivities with densification. These results were used to validate the DEM model [2,3].

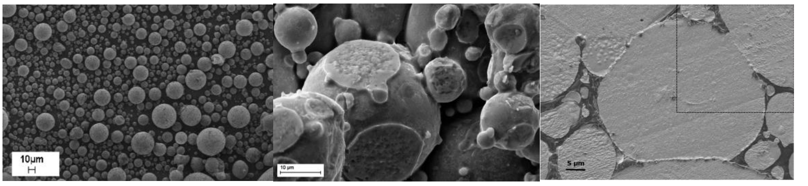

Figure 1. SEM images a) powder morphology, b) fractured surface showing necks and c) grain boundary texture

3. DEM model

An original DEM model, based on sintering geometry where two particles are connected via neck, was presented in [1]. This model was revised by including grain boundary resistance. Additionally, neck-size correction was introduced to compensate for non-physical overlaps at higher densities. The revised DEM model was used to simulate thermal [2] and electrical [3] conduction and evaluate the effective properties of partially sintered porous material with heterogeneous microstructure. The coupled thermoelectric model takes into account the heat generated as result of Joule heating. From the electrical simulation, potential distribution and resulting electric current flow is evaluated by time integrating the following equation:

$$C_i^{el}\dot{V}_i = \sum_{j=1}^{N_i^j} I_{ij} + I_i^{ext} \tag{1}$$

where: C_i^{el} – electrical capacitance of the i^{th} particle, V_i – particle voltage and I_i^{ext} – external current source and I_{ij} – current flow. The temperature evolution in particles is evaluated by time integrating the following heat balance equation:

$$C_i^{th}\,\dot{T}_i = \sum_{j=1}^{N_i^j} Q_{ij} + Q_i^{ext} + \sum_{j=1}^{N_i^j} Q_{ij}^{Joule} \tag{2}$$

where: C_i^{th} – particle heat capacitance, T_i – particle temperature, Q_i^{ext} – external heat source, Q_{ij} – interparticle heat flux and Q_{ij}^{Joule} is Joule heating rate given as follows:

$$Q_{ij}^{Joule} = I_{ij}^2 R_{ij} \tag{3}$$

where R_{ij} is interparticle resistance.

4. Simulation results

The model was validated on the whole sample comprising of 17515 particles. Four geometries with different densities were obtained from hot-press simulation. Similar boundary conditions were assigned to all the geometries. Axial current flow was obtained by prescribing voltage to the top and bottom particles, and the sample was radially insulated to imitate adiabatic conditions as shown in Figure 2. Resulting steady state potential distribution in one of the sample is shown in Figure

3a. Heat generated as a result of current flow resulted in increase in temperature. Homogenous temperature distribution was achieved in the whole sample as represented in Figure 3b. Heating in geometries with different densities is illustrated in Figure 3c. It can be observed that the heating rate increases with increasing density.

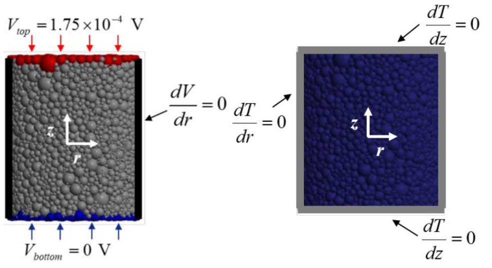

Figure 2. Boundary conditions for the thermo-electric problem

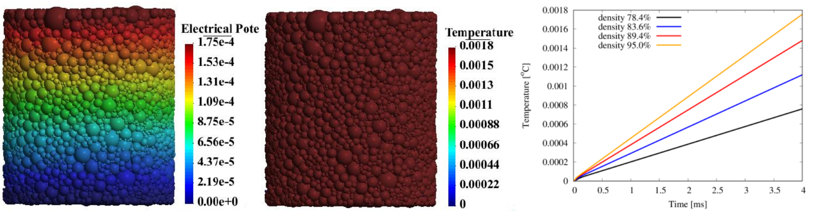

Figure 3. Simulation results a) potential distribution, b) temperature distribution and c) heating in DEM samples with different densitites

5. Conclusion

The coupled thermo-electric model allows to establish a relation between applied current and heating rate for the sintering process. The proposed DEM model can be used for microscopic analysis and can be integrated with sintering models to have a fully coupled thermo-electric-mechanical model for the SPS process.

References

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