Numerical simulation of the entire production route of refractory metals from powder to a sintered metal part

C. Grohs*, N. Reinfried*, A. Plankensteiner*

* Plansee SE, 6600 Reutte, Austria

Abstract

Finite element analyses (FEA) for simulating the powder compaction and sintering commonly has to make use of an initial assumption about the powder filling density and its corresponding distribution in the mold. Therefore, FEA may not be able to predict sintering shrinkage and distortions accurately if an inhomogeneous powder filling density is present in practice which, because of lack of knowledge, has to be approximated by a homogeneous one in the finite element model for the entire powder body in the as-filled state. Futhermore, this also influences in a non-beneficial way the FEA-based predictability of the deformed shape by subsequent hot forming.

The discrete element method (DEM) is an adequate tool for mold filling process simulations. Filling density including spatial gradients as a result of powder manipulating steps can be simulated via DEM by also accounting for filling density influencing actions like mechanical vibration of the mold / powder body assembly. The filling density distribution simulated by DEM then can be used as input in an FEA model for the compaction and de-molding process thus yielding the density distribution of the green part. Based on the latter, inhomogeneous sintering shrinkage can be simulated by an FEA-based sintering shrinkage model this way yields the final shape of the as-sintered component. Finally, the results of the sintering simulations are transferred into an FEA model for hot rolling which yields the final shape of the as-deformed component. The applicability of the whole modeling workflow being applied to a large scale molybdenum component is demonstrated in the present paper.

Keywords

numerical simulation, discrete element method, finite element analysis, powder filling, compaction, sintering, hot rolling

Introduction

The typical steps in the production route of a powder metallurgically produced refractory metal component consist of producing metal powder, powder filling, powder compaction, and sintering as well as subsequent mechanical processing when needed. For example, a sputter target (see Fig. 1) being used for the production of displays represents a rectangular plate with an initial mass of about 900 kg of

the sinter ingot. At the beginning the molybdenum (Mo) powder is filled into an upright standing rubber mold via gravity induced flow. The mold is placed in a steel cage to provide the cuboid geometry.

During and after the powder filling process the powder is subjected to some treatment, including vibrations with an amplitude of some millimeters and a frequency of a few ten Hertz. Then, the mold is sealed with a rubber hose and the powder is compacted by cold isostatic pressing at about 2000 bar pressure. An example for a smaller green part of about 450 kg is shown in Fig. 2. In this picture the curved edges of the plate can be seen which are due to the filling and compaction steps.

Fig. 3 shows two blanks after the sintering process. The density inhomogeneity resulting from compaction is reduced during sintering. This leads to a deformation of the sintered part with less shrinkage where compaction density was higher and more shrinkage at locations of lower green density this way leading to sintering shrinkage of the overall component.

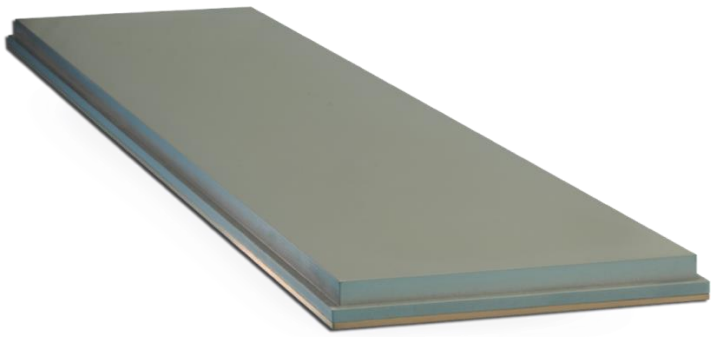


Figure 1: Planar Mo sputtering target on a copper backplate.

Figure 2: Mo green part after powder compaction.

Figure 3: Mo sintered blanks.

Figure 4: Hot rolling of a Mo plate.

Then the sintered part is heated up to above 1000 °C and hot rolled in repeated passes. In Fig. 4 the hot blank leaves the roll stand after the first pass. It is obvious that an unevenly shaped sintered part results into a highly irregular plate in the as-rolled configuration with lots of offcuts resulting thereof.

Simulation Steps

Powder Filling and Void Fraction

For powder filling simulation the open source discrete element modeling (DEM) software LIGGGHTS [1] is used. Based on a measured particle size distribution of standard Mo powder the particles in the simulation are coarse grained with a factor of 150 leading to a simulation model with about 79000 individual particles. DEM-specific material parameters like cohesion, (rolling) friction or restitution are taken from DEM simulations of powder rheometer experiments [2].

The geometry of the mold is included as an ASCII stereolithography (.stl) file which was generated with the open source 3D creation software suite Blender. Fig. 5(a) shows the mold and the filled particles with only three quarters of the model being displayed for visibility reasons. In this simple case the particles were inserted at the whole top surface area and settled uniformly due to gravity. For a more in-depth investigation of the mold filling itself it would also be possible to introduce, for example, a moving nozzle or a hopper in the DEM model for considering effects due to specific characteristics of the filling process.

With the help of CFDEM [3]—which is the coupling of OpenFOAM [4], an open source software for computational fluid dynamics (CFD), with the DEM software LIGGGHTS—the void fraction in the filled mold is calculated as can be seen in Fig. 5(b). Therefore, the mold is divided into small cells (not shown) and 29 points per particle are used to locate each particle in the CFD mesh cells. With the portion of particles in each cell the void fraction is calculated with the value of 1.0 meaning no particles and smaller values giving a higher filling density. Due to wall effects the packing at the boundaries of the mold is not so dense compared to the inner volume which also comes to notice in Fig. 5(b).

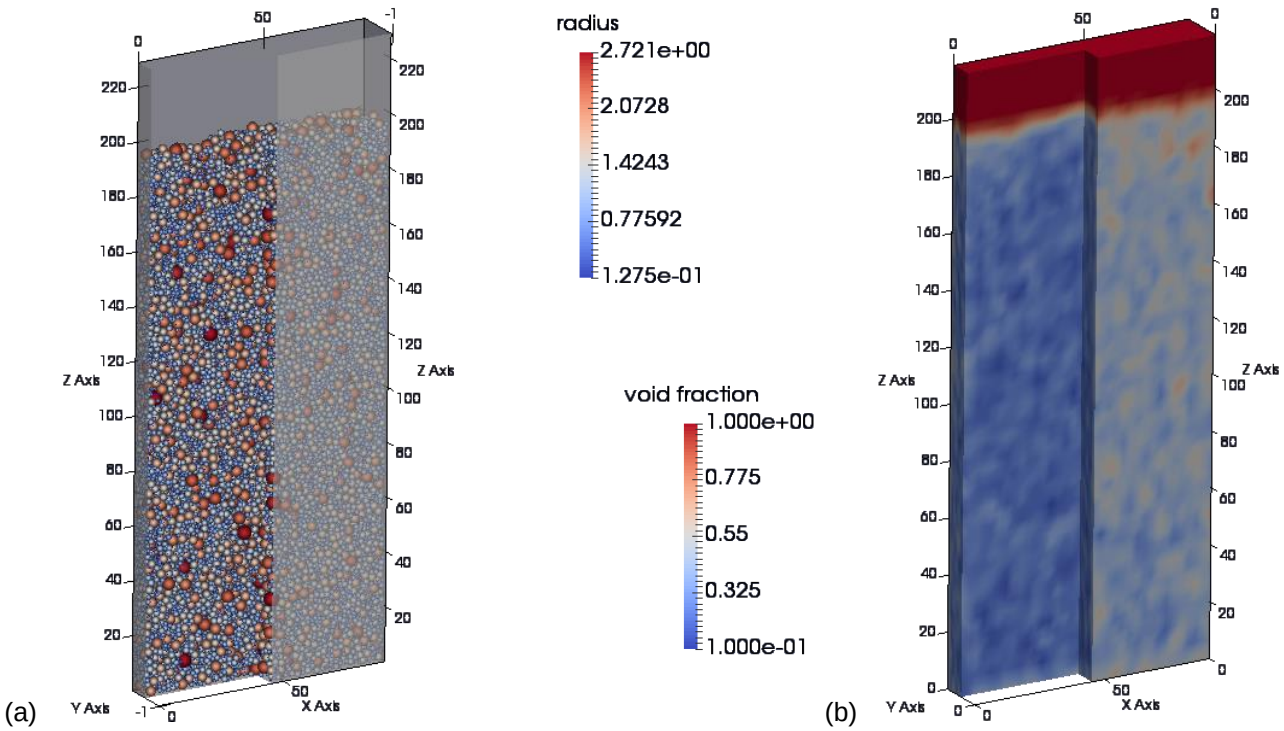


Figure 5: Simulation of (a) particle distribution and (b) void fraction after mold filling in a Mo powder body.

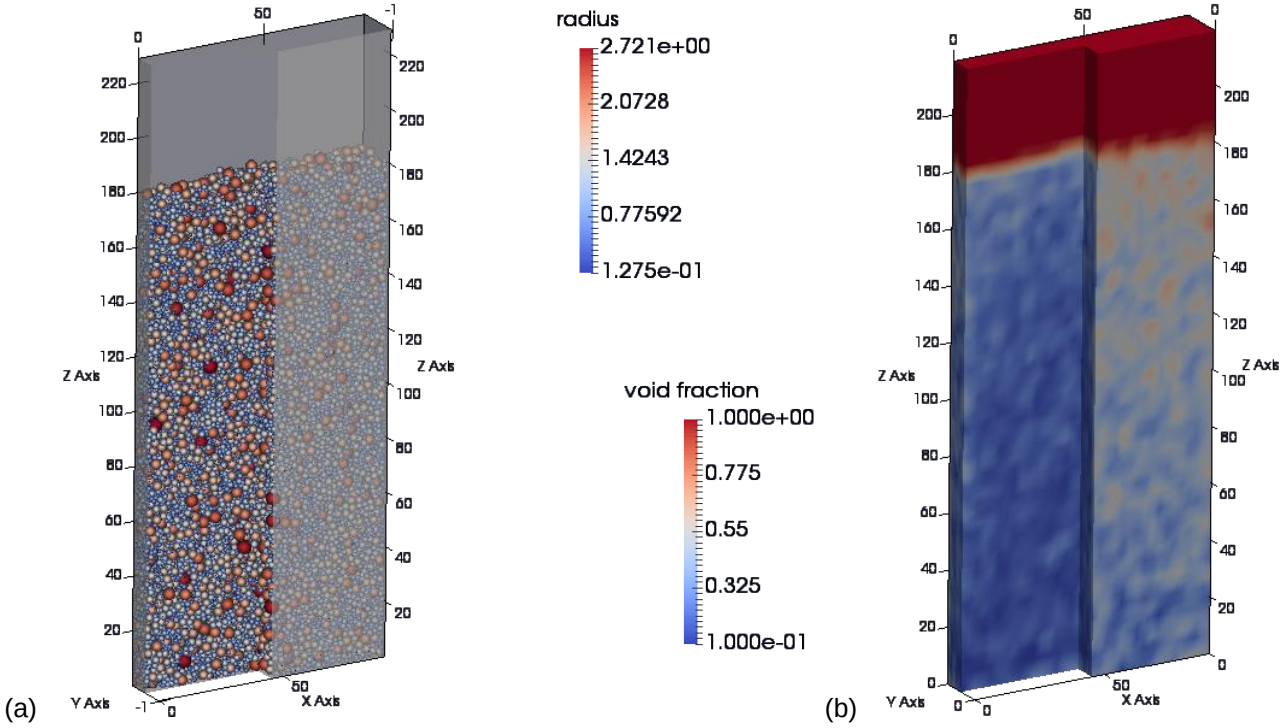


Figure 6: Simulation of (a) particle distribution and (b) void fraction after compaction by vibration in a Mo powder body.

For a further comparison the filled mold in the DEM simulation is vibrated in the vertical direction with a frequency of some ten Hertz and an amplitude of some millimeters typical for the real situation. The resulting particle distribution and void fraction are shown in Fig. 6. Due to vibration compaction the free powder surface descends leading to a higher filling density, i.e. lower void fraction, especially near the bottom of the mold. At this time instant steady state is already reached whereas vibration is still active.

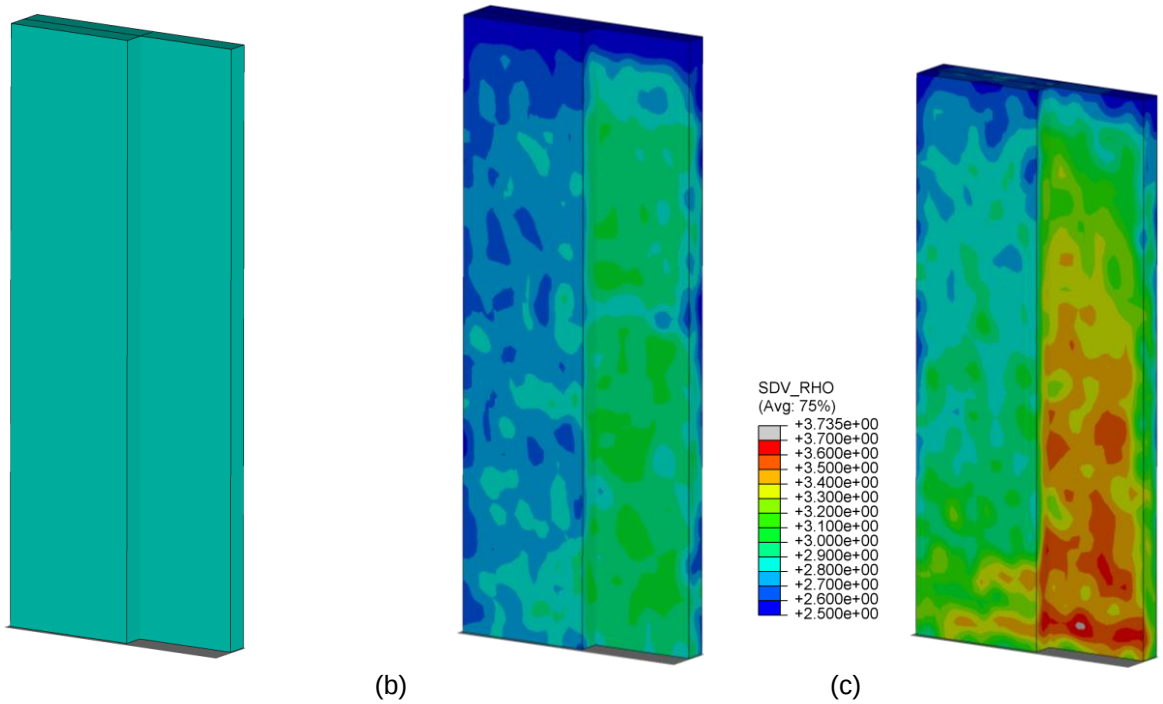
Compaction and Sintering

Further calculations are done with Abaqus FEA [5], a software suite for finite element analysis. Three different simulation models are compared which are listed in Table I to show the influence of powder manipulation on the subsequent processing steps. For the reference model called “ID” an idealized homogeneous filling density is assumed as can be seen in Fig. 7(a). The two other models named “FI” and “FV”, respectively, are based on the previous DEM calculation. Fig. 7(b) shows the density distribution according to Fig. 5 in the as-filled state (FI) while the filling density related to the vibrated powder (FV) of Fig. 6 is represented in Fig. 7(c).

Table I: Simulation models with differently accounted for filling densities

Name	density determination
ID	homogeneous (idealized)
FI	filling calculated
FV	filling and compaction by vibration calculated

Transfer of the filling density distribution to the FEA is done via an Abaqus user subroutine. Therefore, the void fraction of each node of the mesh and its spatial position is taken from the CFDEM simulation and converted to a filling density which is mapped to the new model. The upper part of the particle simulation with zero void fraction is cut away in the FEA model because a lower limit exists for the initial density.



(a) (b) (c)

Figure 7: Calculated density distribution (a) idealized (ID), (b) after filling simulation (FI) and (c) after simulation of filling and compaction by vibration (FV) of a Mo green body

With the calculated filling density distribution cold isostatic pressing (CIP) is simulated. First, by applying gravity the powder is brought into contact with a rigid surface. Afterwards an isostatic pressure on all surfaces is ramped up to the maximum value leading to compaction of the powder body. The used material model is a density-dependent Drucker-Prager cap model with parameters determined by the combination of different simple experiements [6] done with compacted molybdenum test samples.

A nonuniform geometry is achieved at the end of consolidation partly due to friction between the powder body and the rigid surface but mostly because of different levels of filling density, see Fig. 8. Due to higher filling density near the bottom of the green part especially after compaction by vibration (see Fig. 7) the deformation there is less pronounced than in the upper region. This means that the part is thicker at the bottom, relating to powder filling direction, and thinner at the top.

The calculated geometry due to sintering shrinkage is also shown in Fig. 8. For this simulation a simplyfied sintering model is used which computes the shrinkage due to compaction density distribution only. This relationship was also determined by experiments. Due to cold isostatic pressing the erratic filling density levels homogenize to nearly constant compaction density within the whole part at the expense of the geometry. It is worth noting that in contrast when using a rigid die for compaction the geometry of the green part would have exactly the shape of the die but the density distribution would be uneven leading to a deformed sintered part due to shrinkage until similar density is reached everywhere.

The simulation of sintering shrinkage is done with Abaqus/Standard software and in this case, as mentioned before, with a simplyfied sintering algorithm. It would also be possible to use a more sophisticated model for computing sintering [7] which can account for additional influences like, e.g., friction at the contact area of sintered body and support or gravitational forces but for the present aim these influences are of secondary importance and the chosen simple model is sufficient.

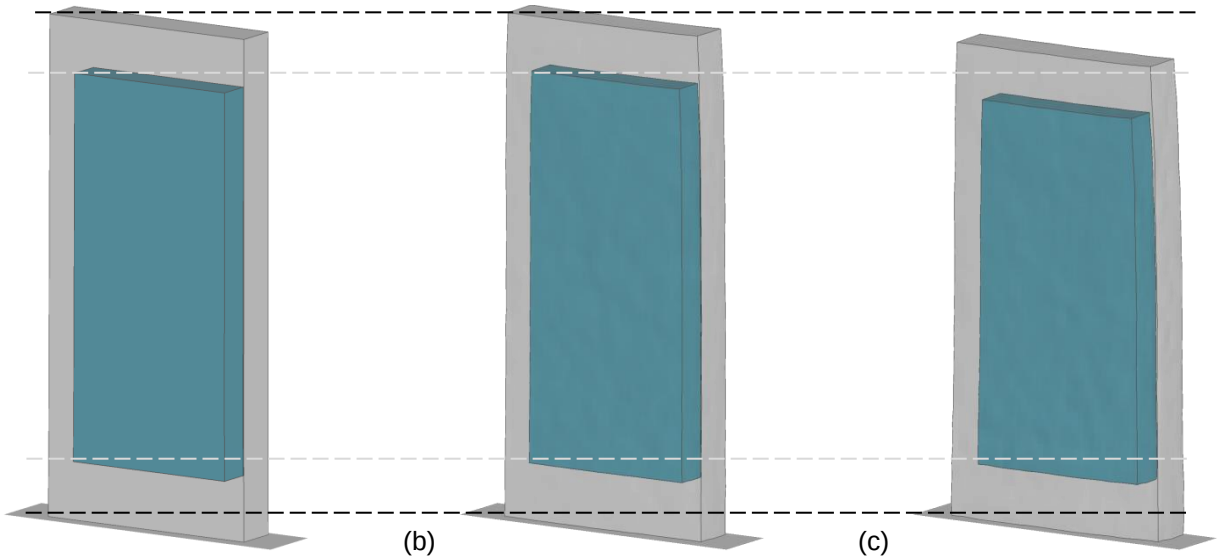


Figure 8: Calculated shape after cold isostatic pressing (grey) and sintering (light blue) for (a) case ID, (b) case FI and (c) case FV. Dashed lines indicate the difference in size for case FV.

Hot Rolling

As the last step in the present work a single pass of hot rolling is simulated. This gives an indication on how powder filling influences the whole further production process. The simulation is done with Abaqus/Explicit software where the results of the sintering calulation, i.e. the deformed geometry, is taken as an input for the rolling simulation. The plate is positioned with one of the long sides as leading edge. Fig. 9 shows a step in the middle of that simulation with the deformable part between two rolls which the latter being modeled as analytical rigid surfaces. The material parameters being used for molybdenum are temperature-dependent and the plate is pre-heated to 1300 °C before start of hot rolling. During the rolling pass temperature changes in the plate are also accounted for.

In Fig. 10 the computed equivalent plastic strain after one pass is shown for the three different cases as defined in Table I. It is obvious that due to the sintered geometry with higher thickness at one end for case FI and especially for case FV the plastic deformation is more pronounced in that area with higher thickness. This leads to increased unsymmetric spreading of the plate in rolling direction. Fig. 11 shows a comparison of the calculated shapes for the three cases after the first pass. On the left hand side of the figure the resulting geometries seen from the top are shown in transparent style while on the right hand side only the upper perimeter of each case are displayed.

Shapes of the cases with constant fill density (blue) and the one with filling only (i.e. no vibration; red) give relatively similar results while the case with filling and compaction by vibration being accounted for leads to visibly irregular deformation. The computed elongation even after the first pass can be seen on the side where the sintered part was thicker. In subsequent passes this would lead to increasing deviation from the desired rectangular shape and therefore to more offcut.

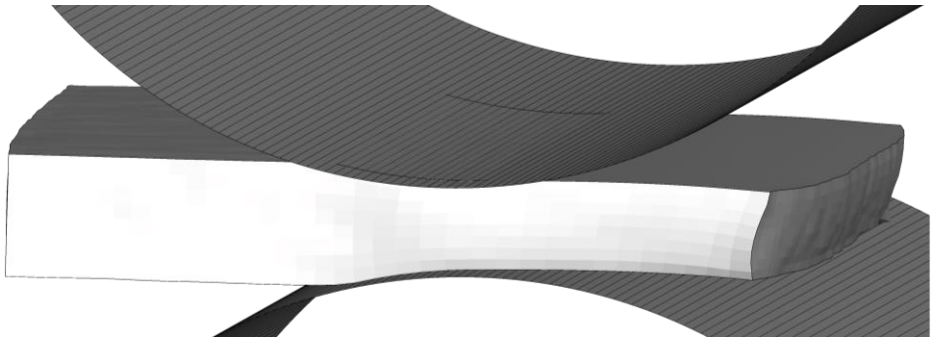
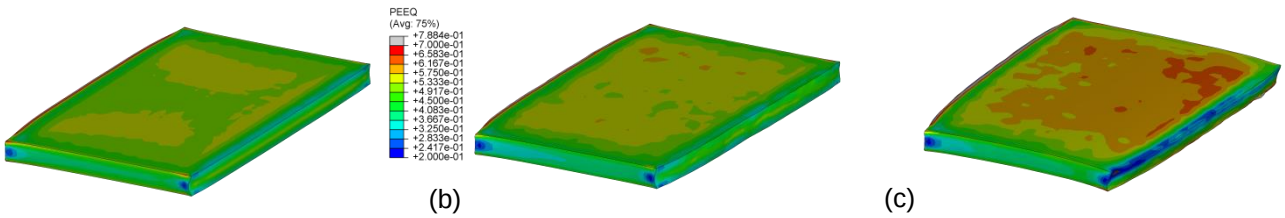


Figure 9: Simulation of hot rolling of a Mo plate.



a) (b) (c)

Figure 10: Calculated shape and equivalent plastic strain after the first pass of hot rolling for (a) case ID, (b) case FI and (c) case FV.

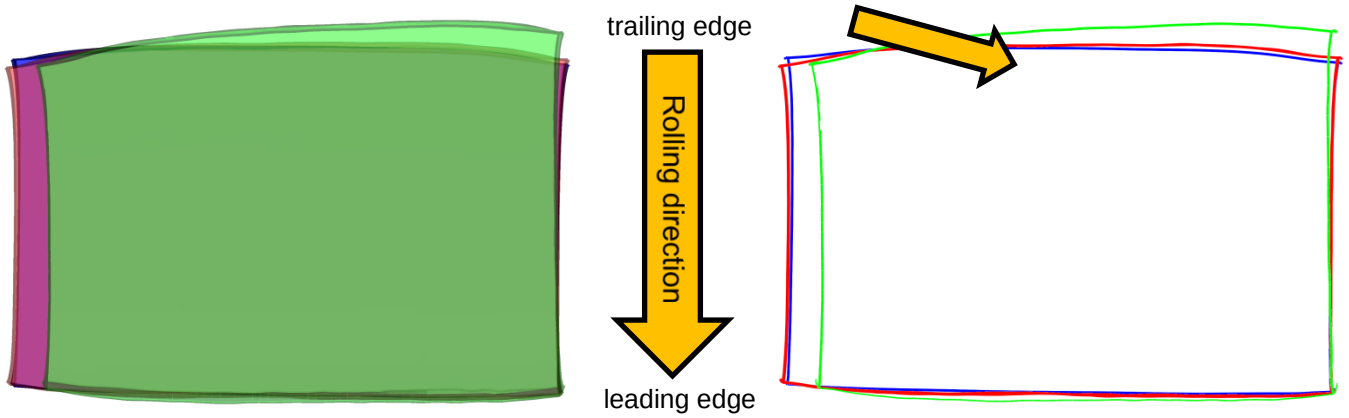


Figure 11: Calculated shapes after the first passage of hot rolling of Mo plate for case ID (blue), case FI (red) and case FV (green).

Summary

With the aid of numerical simulation tools the entire production route of refractory metals ranging from powder filling via sintering to hot rolled parts can be represented. By combining the approaches DEM and FEA along with transfer of results among each other disparate process steps such as powder filling or hot rolling can be linked. It is obvious that each process step influences the subsequent steps and this dependency is also visible within the simulation steps. This way, it becomes possible to study in advance by numerical simulations only e.g. compaction by vibration during the powder filling step and the corresponding impact on the final geometry of a hot rolled plate.

References

1. C. Kloss, C. Goniva, A. Hager, S. Amberger, S. Pirker, Progress in Computational Fluid Dynamics, Vol. 12, Nos. 2/3, pp. 140–152, (2012)
2. C. Grohs, C. Schäfer, U. Schleinkofer, A. Plankensteiner, Proceedings World PM2016, Hamburg, (2016)
3. C. Goniva, C. Kloss, N.G., Deen, J.A.M. Kuipers, S. Pirker, Particuology, DOI 10.1016/j.partic.2012.05.002, (2012)
4. OpenFOAM Foundation, https://openfoam.org, (2016)
5. Dassault Systems, www.3ds.com, (2016)
6. A. Plankensteiner, C. Feist, C. Grohs, K. Huber, L.S. Sigl, Proceedings World PM2010, Florence, (2010)
7. A. Plankensteiner, L.S. Sigl, H. Kestler, Pulvermetallurgie in Wissenschaft und Praxis, Band 27, pp. 255–272, Fachverband Pulvermetallurgie, Hagen, (2011)