NUMERICAL ASSESSMENT OF FAILURE-CRITICAL STRESS-STATES IN A POWDER-COMPACTED BI-MATERIAL COMPONENT

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Abstract

The present work aims at assessing critical stress-states which occur during double pressing of disk-shaped tungsten/molybdenum green bodies. The powder body is composed of a thin W-layer on top of a Mo-substrate. Experimental evidence shows that degradation of the green body actually occurs during pressing by crack formation in both bulk materials and by debonding at the W/Mo-interface. This behaviour is attributed to (i) differences in the mechanical properties of the Mo- and W-powders and to (ii) the two-step compaction process where homogeneous powder filling into an auxiliary die with subsequent pre-compaction is followed by a die-compaction step. The flow and re-arrangement of powder-particles in the auxiliary die is modelled by means of the discrete element method (DEM). The final pressing step of compaction and ejection is simulated by a finite element based (FEM) model whose initial conditions are set by the DEM results.

After an initial settlement process of the powder, the formation of a pronounced macroscopic shear-plane is predicted by DEM. The subsequent FEM calculation forecasts considerable plastic deformation in the tungsten layer during ejection of the component and further plasticity peaks at the intersection of the tungsten layer with the shear-plane. The predicted shape of the bi-material interface of the final powder compact matches well with actual observations. Hence, the DEM-FEM approach is considered to model the two-step compaction process correctly, including powder transfer, powder compaction and ejection. The DEM-FEM model is currently being used to identify and evaluate failure-prone conditions for various processing plans.

Keywords

Finite Element Method, Discrete Element Method, Powder Transfer, Powder Compaction, Crack;

Introduction

Molybdenum, tungsten and their alloys are refractory metals which are widely used in technical high-end applications where high-temperature strength, high thermal conductivity, low thermal expansion as well as high resistivity against aggressive media are key properties. Rotating X-ray targets for human medical diagnostics are among the most prominent examples for such applications. In modern spiral scan computer tomography applications, a focused and pulsed electron beam is placed onto a focal track enabling the emission of X-ray. This process, however, is accompanied by the generation of a considerable amount of heat with specific heat fluxes on the order of 10,000 W/mm^2, thus belonging to the highest ones in today's technical applications. In order to limit peak temperatures to app. 2,500°C, disk-shaped targets have to be rotated and are typically made from a molybdenum (Mo) based alloy for the target cup and a tungsten (W) based alloy for the focal track layer. The target

cup ensures the mechanical integrity of the system during spinning of up to 200 Hz at target diameters of up to 200 mm. In addition, it serves as the heat storing or heat conducting component of the target depending on whether passive cooling via thermal radiation or active cooling is employed for the X-ray target system. Thus, it is clear that rotating X-ray targets have to withstand exceptional thermo-mechanical loads in a typical life time of 100,000 electron beam exposures.

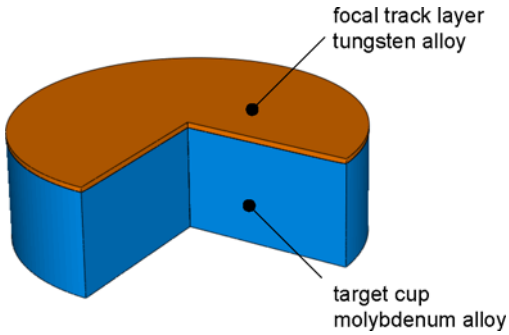

Fig. 1: Sketch of a green body of a rotating bi-material X-ray target of 140 mm in diameter using tungsten alloy for the focal layer and a molybdenum alloy for the target cup section.

The powder metallurgical (PM) production route of such bi-material disk-shaped targets starts with the co-compacting of the Mo-body and the W-layer to form a green body (Fig. 1). The latter is subsequently consolidated by free sintering and hot forging to obtain the required mechanical material characteristics. This procedure generates a bi-material interface with outstanding mechanical integrity and thermal conductivity which both are of primary importance for the power rating of the target.

Even though these components are manufactured in serial production, debonding between the focal track and the target cup section right after ejection of the green body out of the die has been observed in some targets, see Fig. 2. An integrative modelling and simulation approach of die pressing by employing the discrete element method (DEM) and the finite element method (FEM) is devised in order to identify potential reasons for the observed phenomena and to derive an optimized set of processing parameters.

Modelling of the die filling and powder compaction procedure

The specific die filling and compaction procedure adopted for such PM components consists of several steps, see Fig. 3: First the Mo powder is filled into an auxiliary die of up to 200 mm in diameter and subsequently pre-compacted at a low pressing force of several 100 N in order to form a powder pre-compact with a planar upper surface. In the following step, W powder is filled onto the top surface of the Mo pre-compact using the same procedure as described above. The auxiliary die containing the bi-material pre-compact is then transferred to the hydraulic press and the pre-compact is inserted into the die by lowering the lower punch. It is worth noting that the radial clearance between the pre-compacted powder body and the die is about 0.5 % or less of the radius of the die. After powder compaction with pressing forces of several 1000 kN, the pressing force is reduced to a load of several 100 kN and kept constant during the subsequent ejection of the green body. The processing sequence is completed by unloading the punches.



Fig. 2: Perspective view onto the bi-material interface of a W layer of an X-ray target. (a) The W-layer is debonded from the Mo target cup during the powder compaction process chain and is shown in an as-sintered condition. Chemical etching has been used to completely remove the scrap Mo from the W layer. (b) A geometrical discontinuity with a height of 0.25 mm can be observed in the as-sintered condition corresponding to a height of 0.30 mm in the as-pressed condition.

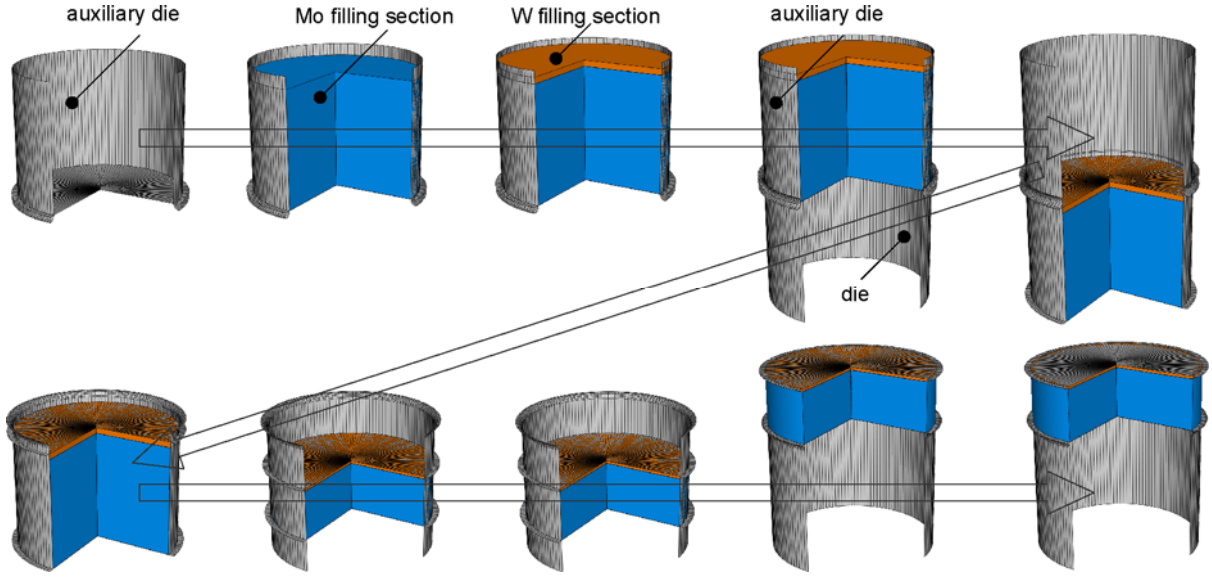

Fig. 3: Schematic view on the processing plan for die filling and compaction of an X-ray target green body of 140 mm in diameter: auxiliary die → filling of Mo powder, pre-compaction → filling of W powder, pre-compaction → transferring auxiliary die and bi-material powder pre-compact to press directly above die → inserting powder pre-compact into die → removal of auxiliary die → pressing → load reduction → ejection → unloading.

The DEM-based modelling approach aims at simulating the behavior during insertion of the bi-material powder pre-compact and the very early stages of pressing during which the radial clearance between the die and the powder pre-compact vanishes. This regime is characterized by very small loads where the micro mechanics of the powder are better described by the DEM approach rather than by continuum mechanics based FEM models. Furthermore, the DEM model adopts a full 3D representation of the morphology of the powder material.

The subsequent FEM-based modelling accounts for the powder compaction and ejection process and adopts an axisymmetric 2D model. Tool surfaces contacting the powder body are assumed to be rigid and corresponding frictional forces are accounted for by a Coulomb friction law. Within the FEM approach perfect bonding at the bi-material interface is assumed.

Both the DEM and FEM approach are employed consecutively with the deformed shape of the powder pre-compact and particularly geometrical imperfections serving as the primary variables to be transferred.

Micro and macro mechanical material description

It is generally agreed that micromechanical approaches are most suitable to describe die filling and powder transfer processes, see e.g. [1], [2], [3]. This is mainly due to the effect that the behaviour of loose powder under primarily gravity induced loading conditions cannot be

concisely described by a phenomenological macroscopic material model. Even recent developments in macroscopic constitutive modelling such as the single surface yield plasticity approach by [4] tend to focus on failure-prone conditions during compaction and ejection stages rather than on powder filling and transfer. The explicit consideration of individual powder particles or their agglomerates in approaches such as the DEM can account for micro-mechanisms such as grain translations and rotations, inter-particle contacts including frictional effects as well as particle-tool surface interactions. Although some plasticity theories such as those based on Cosserat continua [5] are capable of handling translational as well as rotational degrees of freedom, they still exhibit a macroscopic and phenomenological character. Consequently, they are limited with respect to their applicability to die filling and powder transfer.

In the framework of the present work the generic molecular dynamic (MD) code **LAMMPS** [6] is employed. The code is capable of modelling atoms, molecules or particles in general from atomic up to the continuum scale. The field of application ranges from soft materials such as polymers to hard solid-state materials such as metals and granular systems. In the present case its capabilities in modelling granular materials are exploited by means of its specific granular module which is specifically extended in the framework of the **LIGGGHTS** package [7], thereby offering the functionalities of the discrete element method (DEM). In particular, **LIGGGHTS** accounts for (i) interactions between individual particles (e.g. Hertzian contact, friction, etc.), (ii) interactions between particles and rigid walls, and (iii) interactions between particles and the ambient including gravity and viscous forces exerted from the surrounding fluid. With respect to discretization of the granular material, **LIGGGHTS** uses spherical particles equipped with translational and rotational degrees of freedom which can be arranged to larger non-spherical particles or agglomerates by means of fixed bonds. On the other hand, tool-surfaces can be represented by granular walls, analytically describable and triangularized surfaces, respectively. In general, these surfaces can follow prescribed rigid-body motions. Symmetric and periodic boundary conditions can be applied in case of analytical surface definitions. Triangularized surfaces can be directly derived from imported CAD data. Finally, successful attempts have been made to couple the DEM features of **LAMMPS / LIGGGTHS** with a CFD-based description of the surrounding fluid using **OpenFOAM** [8]. This allows for full coupling of fluid and particle dynamics.

For the present study the DEM model is used to predict the powder transfer after removing the auxiliary die, i.e. when the radial gap between the pre-compact and the wall of the pressing die is being filled. The simulation starts with the powder pre-compact being placed within the auxiliary die. Powder-transfer is captured by instantaneously removing and adding the surfaces representing the auxiliary die and pressing die, respectively. Even though the physical problem is axisymmetric with respect to the macroscopic setting (geometry of powder pre-compact and tools), DEM requires that the problem has to be captured by a three-dimensional model. In this context it suffices to model a 3D sector of finite angular extension. As a simplification, the resulting wedge-like shaped body is represented by a cubic body of appropriate width with respect to the chosen particle size. Periodic boundary conditions are applied to the sectional planes. Particle sizes are assumed in the range between 1.0 and 2.0 mm resulting in a total of app. 20,000 spherical particles. The latter are assumed as elastic exerting frictional and cohesive forces to other particles and tool-surfaces. In the present case only particle dynamics are accounted for and viscous forces from the air are modelled by simplified velocity-dependent damping forces.

On the other hand the constitutive material characteristics for the FEM-based compaction and ejection simulations are modelled for both powder materials by a combined Drucker-Prager/cap (DPC) plasticity model, which represents a macro mechanical phenomenological material description, see e.g. [9] and [10] for a detailed description. The cap yield surface of the model describes the nonlinear material response for stress states of high triaxiality and is

calibrated using instrumented die experiments. The Drucker-Prager yield surface, commonly referred to as shear-failure surface, captures the low triaxiality stress states and is usually assessed by uniaxial compression tests and the Brazilian disk test, see Fig. 4.

The constitutive state within a granular material primarily depends on the material density in a macroscopic sense. Consequently, the latter quantity is introduced as an internal variable in the model and evolution of both yield surfaces is described by appropriate hardening laws. A graphical representation of this evolution as a function of density is displayed in Fig. 5 for selected Mo and W powders. Clearly, the yield surfaces enclosing the elastic domain expand with increasing density thereby accounting for the respective increase in shear and compressive strength. The reversible, i.e. elastic, fraction of the material response is described by an isotropic nonlinear, i.e. density-dependent relationship.

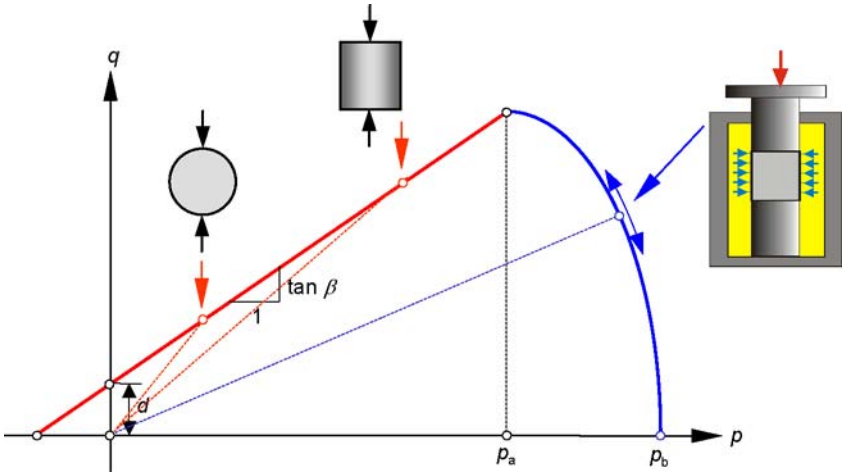

Fig. 4: Representation of the combined Drucker-Prager/cap yield surface in the hydrostatic – deviatoric stress space p – q. Typical stress paths for a Brazilian disk test, a uniaxial compression test, and an instrumented die experiment are indicated schematically.

In the inelastic regime favorable stress paths during compaction and ejection follow the cap yield surface describing irreversible material compaction of low risk for failure-prone conditions. On the other hand, stress-paths hitting the Drucker-Prager shear failure surface indicate an inelastic material response which is accompanied by a decrease of density. Such material response can be regarded responsible for later crack formation and, consequently, should be avoided by appropriate adaption of the compaction and ejection parameters. It should be noted that the present model is only capable of indicating stress-states of potential risk for crack nucleation but cannot predict crack-propagation.

Debonding at the interface between Mo and W

As described above, the bi-material powder pre-compact is inserted into the die by employing a diameter of the powder body being slightly smaller than the die. At this stage the DEM approach is introduced to simulate the powder-settlement from the removal of the auxiliary die and the resulting radial gap, see Fig. 6. For the component under consideration the overall filling height is 101 mm, the diameter of the powder pre-compact is 139.50 mm and the diameter of the die is 140 mm.

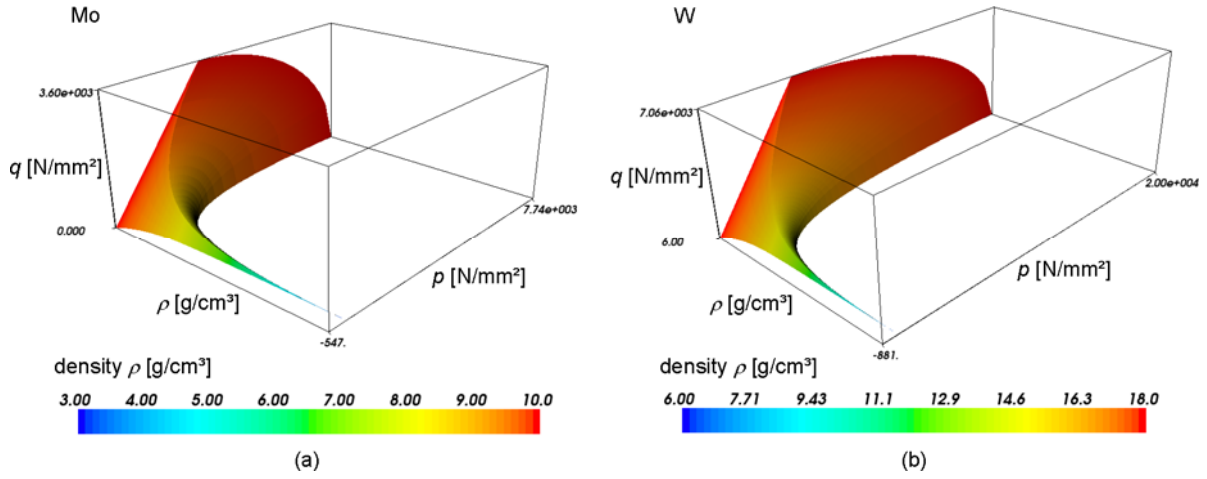

Fig. 5: 3D representation of the density dependent Drucker-Prager/cap yield surface for (a) molybdenum and (b) tungsten, respectively, as calibrated on instrumented die experiments as well as uniaxial compression tests and Brazilian disc tests, respectively.

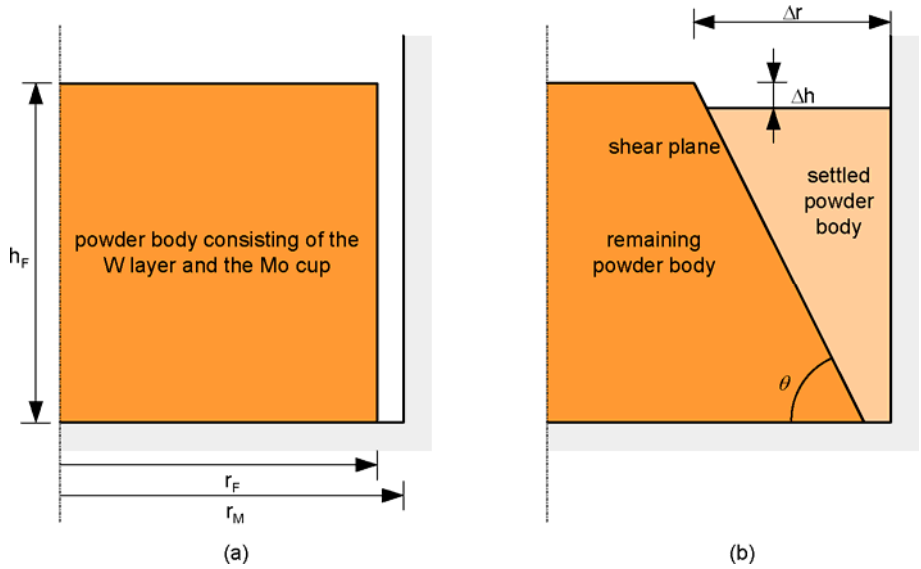

Fig. 6: Sketch of the idealized settlement process at outer zone of the powder body due to the presence of a radial clearance: (a) initial configuration with radial gap, (b) settled configuration after powder-transfer.

In order to compensate the initial radial clearance prior to or at the very beginning of the pressing operation, a settlement of the powder body in the outer region is expected to affect a volume of about 11.1 cm^3.

The powder-packing before removal of the auxiliary die is depicted in Fig. 7 (a) representing the initial stationary state. Fig. 7 (b) shows the numerically obtained final deformed configuration with the contour levels representing the magnitude of the individual particle-displacements relative to the initial state. Obviously, the largest displacements are predicted

for an inverse cone-shaped section at the outer region of the powder pre-compact. Within this section nearly no displacement gradient is observed which can be interpreted as a rigid-body motion. On the other hand a fairly steep displacement gradient develops across a plane inclined at approximately 70° which indicates localization of the displacement field in terms of a shear plane which tends to separate two distinct individually moving volumes: a quasi-static truncated cone in the interior and an inverse cone undergoing a rigid body motion ensuring the cavity resulting from the initial radial gap to be entirely filled.

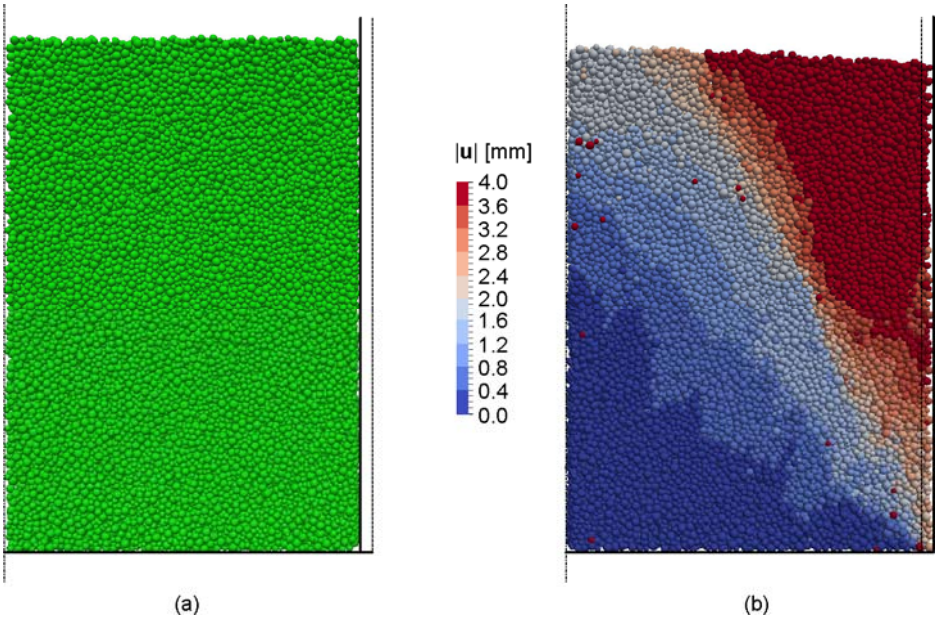

Fig. 7: DEM-model for the simulation of the initial powder-transfer: (a) initial powder package within the auxiliary die and (b) deformed stationary state in the pressing die with contours showing the magnitude of the total relative displacement vectors.

The effect of localization in terms of relative tangential displacements of these bodies along the shear-plane is not yet very pronounced and a vertical offset of the top surfaces cannot be yet identified. This is due to the fact that within the DEM simulations the particles - for the sake of numerical efficiency - are orders of magnitudes larger than the real powder-grains, such that the ratio of particle size and gap size is altered. Nevertheless it can be expected that for further particle refinement localization becomes more pronounced. Consequently, one can consider the rearrangement through powder-transfer to happen in an idealized manner as shown in Fig. 6 (b).

By explicitly assuming a cone-shaped shear plane inclined at an angle of $\theta = 70°$ as well as complete filling of the gap volume results in a settlement depth of about $\Delta h = 0.93$ mm. In this case the shear plane intersects the initial top surface at a radial distance measured from the outer perimeter of $\Delta r = 36.76$ mm, compare Fig. 6 (b).

The FEM approach is now adopted to evaluate the plastic activity of the individual powder sections with the initial conditions for the settlement given in Fig. 8. While the compaction step is highly compressive with high stress triaxiality, the ejection stage is characterized by lower stress triaxilities with some regions of the green body undergoing even tensile loading. Generally, stress states on the shear-failure surface should be avoided. This requirement is hardly fulfilled at the cylindrical free surface of the powder body which contacts the die due to friction. In particular, the ejection of the component induces considerable plastic activity even in the entire volume of the W layer due to pronounced tensile stressing, see Fig 9 (a, b). In contrast, almost the whole Mo powder section remains elastic during the ejection process, compare Fig. 9 (a, b). In particular, the settlement process prior to compaction gives rise to a

pronounced geometric discontinuity after completion of processing which is accompanied by additional plastic yielding in a localized region. From an application point of view such a discontinuity at the interface between the focal track and the target cup should never be located in the heat affected zone of the electron beam otherwise severe damage of the X-ray target could occur. Fig. 9 (c) shows a comparison between the predicted and measured thickness variations of the W layer as a function of radial position showing good agreement. Modifications of the pressing schedule can now be readily used to minimize (i) plastic yielding in the focal track layer and (ii) formation of interfacial discontinuities at the bi-material interface while characteristics of the powders need not to be changed.

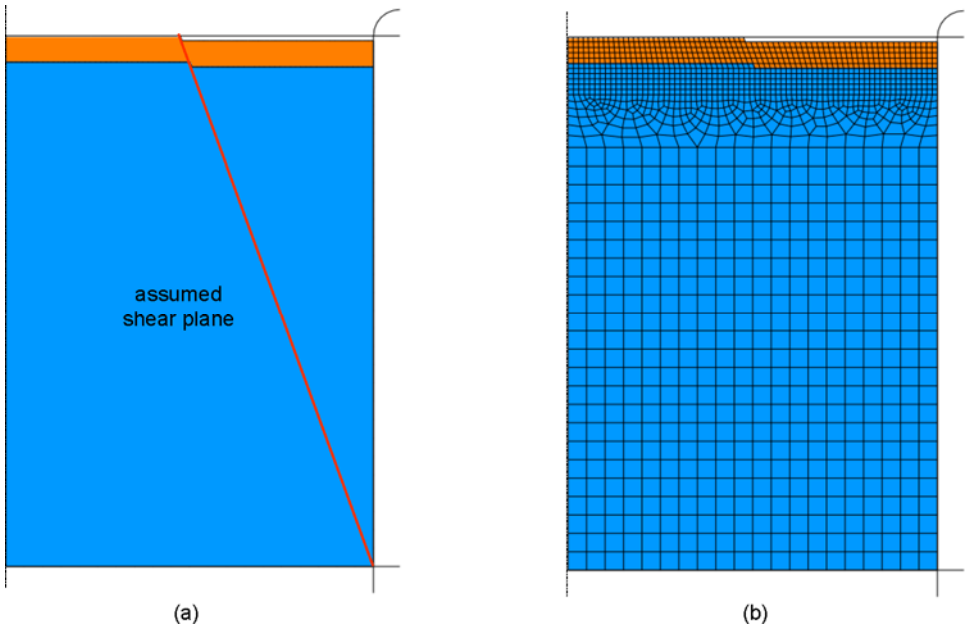

Fig. 8: (a) Geometrical representation of powder body and tool surfaces, and (b) corresponding FEM discretization of the bi-material powder pre-compact with a settled region separated by an explicitly assumed imaginary shear plane.

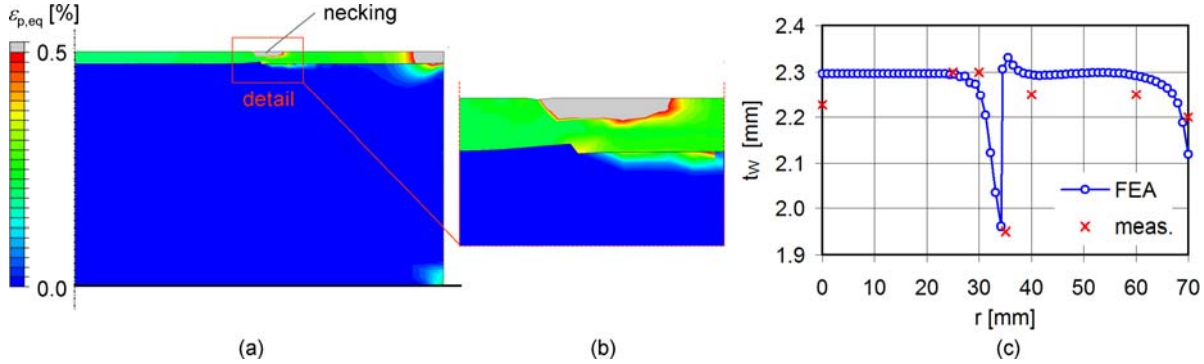

Fig. 9: Results from FE-analysis: Predicted equivalent plastic strain from plastic activity on shear-failure surface for (a) entire green-body and (b) close-up in region near shear-plane as accumulated through the ejection process and displayed after complete unloading; (c) Predicted (blue) and measured (red) thickness distribution in radial direction for the W layer of an X-ray target in the as-pressed condition.

Conclusions

Powder compaction of disk-shaped bi-material compounds made of Mo and W alloys represents an integral part of the production route of X-ray targets used in medical X-ray imaging. Because of the contrast in mechanical characteristics of the Mo and W-powders and due to specific multi-step operations during powder filling and compaction, geometric discontinuities appear in the W/Mo-material interface which enforce interfacial debonding. An integrated DEM-FEM modelling approach is adopted to simulate powder transfer behaviour and the elastic-plastic behaviour during compaction and ejection. Thereby the relationships between processing parameters and the evolution of stresses and plastic strains are identified over the loading history. It is shown that this approach can predict the regions of localized plastic yielding which is observed in the W layer during the ejection phase of pressing. Since there is good quantitative agreement with experimental observations, the DEM/FEM approach can be used for further process optimizations.

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