Multi-grain finite element model for studying the wire drawing process

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Abstract

Wire drawing of tungsten wires leads to a special microstructure which is characterized by elongated curled grains and a sharp (110) texture. At this moment the computational power does not allow to simulate this deformation process by taking into account the whole grain structure. Therefore a cubic unit cell that takes into consideration the grain structure of the wire was selected and modelled in detail to study the features in a qualitative way. Individual grains of the unit cell are described within the framework of continuum crystal plasticity. The boundary conditions are idealised wire drawing conditions. Simulations were performed to study the evolution of the texture and the curling effect. They show that the presented model along with the constitutive theory of crystal plasticity is able to predict texture development, grain elongation and the curling of grains with an initially sharp (110) texture.

Keywords: Tungsten; Texture; Crystal plasticity; Finite element; Viscoplasticity

1. Introduction

In the lightening industry tungsten wires with a diameter of 40 µm are fabricated to coil them and use them as lamp filaments. To obtain such small diameter swaged tungsten rods with a diameter of several millimetres are drawn through several drawing dies. During this severe deformation process longitudinal cracks can occur which are known as splits [1] and which are of intergranular nature.

To gain more insight in the reason for splitting it is necessary to have a closer look at the microstructure and its changes during wire drawing. Originally equiaxed grains get highly elongated in the longitudinal section. Furthermore, the BCC tungsten grains rotate leading to a sharp (110) fibre texture [1]. Tungsten wires with such a well established (110) texture present a heterogeneous microscopic deformation characterized by curling (bending) of the grains around the wire axis in the transverse section [2]. As successfully explained by Hosford [3], the stress required for axially symmetric flow of individual crystallites is higher than the stress required for plane strain. Therefore, during wire deformation grains develop an elliptical shape in the wire cross section where the major axes of the ellipses are randomly oriented. This fact enhances mutual accommodation of the grains during the deformation process and creates a pattern in the wire cross section known as “Van Gogh sky structures”. These structures were successfully modelled by Gil Sevillano et al. [4] using a geometrical model approach.

The aim of this work is to establish methods to predict the above described microstructural changes during wire drawing. The drawing process itself has often been simulated with macroscopic models. They allow to study for example the influence of the process conditions on the first order residual stresses [5] but not surprisingly they fail in the description of microstructural changes. To be able to predict these features the grain structure has to be represented and described with crystal plasticity (Section 2). As several thousands of grains build up the cross section of the wire, it is not feasible to discretize
the whole wire. Instead the presented models are based on the cubic unit cell with periodic boundary conditions (Section 3). The developed 3D model is applied to study the evolution of texture during wire drawing (Section 4.1) and the 2D model predicts the curling phenomenon (Section 4.2).

2. Formulation of crystal plasticity

Tungsten grains are modelled with crystal plasticity [6–8]. This theory takes into account the orientation of the lattice in each grain and describes the result of the movement of dislocations (namely slip) in a continuum way. This means that plastic deformation is the result of continuous shearing (slip) along various well-defined lattice planes. A slip system is defined by the unit normal \( n^{(s)} \) to the slip plane and the unit vector \( s^{(s)} \) in the slip direction. The rate of change of the Schmid tensor \( F_{ij} \) posed into parts due to lattice deformation (*) and plastic slip (p) where

\[
F_{ij}^{(*)} = F_{ij}^{(p)} + F_{ij}^{(s)}.
\]

The slip system normal and slip direction in the deformed configuration are defined as \( m^{(s)}_{ij} = m_{ij}^{(s)} F_{ij}^{-1} \) and \( s_{ij}^{(s)} = F_{ij}^{(s)} s^{(s)} \), respectively.

The rate of the stretching tensor \( D_{ij} \) can be also decomposed into parts due to lattice deformation (*) and plastic slip (p)

\[
D_{ij} = D_{ij}^{(p)} + D_{ij}^{(s)}.
\]

The flow rule based on Schmid’s law is determined by the Schmid tensor \( P_{ij}^{(s)} \) and the shear rate \( \dot{\gamma}^{(s)} \) on the slip system \( s \) in form of a power law

\[
D_{ij}^{(s)} = \sum_{s=1}^{n} P_{ij}^{(s)} \dot{\gamma}^{(s)}, \quad P_{ij}^{(s)} = \frac{1}{2} (s_{ij}^{(s)} m_{ij}^{(s)} + m_{ij}^{(s)} s_{ij}^{(s)}),
\]

where \( \tau^{(s)} \) stands for the resolved shear stress on the slip system \( s \), i.e.,

\[
\tau^{(s)} = s_{ij}^{(s)} \sigma_{ij} m_{ij}^{(s)} = P_{ij}^{(s)} \sigma_{ij},
\]

\( \dot{\gamma}^{(s)} \) denotes a reference shear rate and \( m \) the material rate sensitivity, where \( g^{(s)} \) means the slip system hardening. The value of each \( g^{(s)} \) for \( \gamma = 0 \) (\( \gamma = \int \dot{\gamma}^{(s)} \, dt \)) has to be specified and denoted with the symbol \( \tau_{0} \).

The strain hardening obeys the following evolution law:

\[
\dot{g}^{(s)} = \sum_{\beta} h_{s\beta} \dot{\gamma}^{(\beta)}
\]

with the hardening matrix \( h_{s\beta} \), where \( h_{s\beta} \) stands for self-hardening on system \( \beta \) while \( h_{s\beta} (x \neq \beta) \) describes the latent-hardening rate of system \( x \). A simple form is used for \( h_{s\beta} \) [6]

\[
h_{s\beta} = h(\gamma) = h_{0}\text{sech}^{2} \frac{h_{0}(\gamma)}{\tau_{s} - \tau_{0}} \quad (\text{no summation over } x),
\]

where \( h_{0} \) represents the initial hardening rate and \( \tau_{s} \) stands for the saturation strength. The latent hardening modulus is given by

\[
h_{s\beta} = qh(\gamma) \quad (x \neq \beta)
\]

with the latent hardening parameter \( q \).

Crystal plasticity is implemented as a user material subroutine UMAT [9] in the finite element code ABAQUS.

3. Finite element modelling

3.1. Cubic unit cell

The computational power available nowadays still does not allow us to simulate the complete wire. Alternatively, a unit cell is built up to analyze the evolution of the microstructure during the deformation. The unit cell with its polycrystalline morphology is created using a software module of Palmyra developed in a collaboration between MatSim and the Fraunhofer Institute for Mechanics of Materials. The program provides 3D Voronoi tessellations on a periodic cubic mesh.

The cubic unit cell for the 3D analysis contains 10 grains and \( 20^3 \) cubic finite elements (Fig. 1(a)). For the detailed curling analysis a 2D geometry is sufficient. The size of the mesh is \( 50^2 \) elements and it contains 12 grains (Fig. 1(b)). Each grain of the unit cell possesses a different crystal lattice orientation and obeys the single crystal plasticity constitutive equations. The initial orientation of the grain is prescribed to represent the desired initial texture. More details concerning the lattice orientations are given in Sections 4.1 and 4.2.

3.2. Boundary conditions

The applied boundary conditions correspond to idealized wire drawing conditions. Material points at the wire axis experience a deformation very close to these conditions. Furthermore, we use periodic boundary conditions to minimize the constraint effects. This means that the displacement vectors of two equivalent points a and b are coupled by the macroscopic deformation gradient \( \mathbf{F}_{ij} \) [10]

\[
u_{i}^{b} - u_{i}^{a} = \mathbf{F}_{ij} \left( x_{i}^{b} - x_{i}^{a} \right) - \left( x_{i}^{b} - x_{i}^{a} \right),
\]

where \( x_{i}^{b}, x_{i}^{a} \) indicate the position of a point pair in the non-deformed configuration. The deformation gradient \( \mathbf{F}_{ij} \) for ideal wire drawing conditions as a function of time \( t \) has the following form:
3.3. Material parameters

BCC materials have three slip system families containing 48 slip systems (Table 1). All three slip system families are taken into account in our simulations. The initial yield stresses for the slip families are selected to satisfy $\tau^I < \tau^{II} < \tau^{III}$ with following ratio, 1:1.3:1.5.

Approximate hardening parameters are used, since the principles of curling should depend more on the lattice type and the available slip systems than on the absolute magnitudes of the stresses and the detailed hardening behavior. For the same argument, the latent hardening parameter $q$ is set to one so that the Taylor isotropic hardening is imposed.

\[
\mathbf{F}(t) = \begin{bmatrix} -kt & 0 & 0 \\ 0 & -kt & 0 \\ 0 & 0 & F_{33} \end{bmatrix},
\]

where $k$ is the compression velocity. The material is free to expand in wire axis direction so that the component of expansion $F_{33}$ is only restricted to hold the force equilibrium.

4. Results

4.1. Evolution of the $\langle 110 \rangle$ fibre texture and incipient curling in a 3D model

The 3D model is applied to simulate the evolution of a multigrain microstructure with initial random orientation distribution of the crystal lattice. Fig. 2 demonstrates how the grains elongate and start to curl with increasing deformation. These findings correspond to the experimental observations. It is also well established, that wire drawing produces a $\langle 110 \rangle$ fibre texture. To evaluate the prediction of our model, the time evolution of all equivalent $\langle 110 \rangle$ directions are extracted and projected into pole figures. The standard stereographic projection with the centre of the pole corresponding to the wire axis direction is used. Note, that we do not distinguish the sign of a direction vector. For instance $[011]$ and $[01\bar{1}]$ are considered as the same direction.

In Fig. 3 the pole figures are shown for three particular material points corresponding to different grains. Their notation and position are recorded in Fig. 2. The initial orientation of the projected $\langle 110 \rangle$ directions are denoted with cross “×” and as the lattice rotates during the applied
deformation, the projected directions draw continuous lines in the pole figure (see Fig. 3).

Pole Fig. 3 (a) and (b) manifest the most characteristic behavior. The $h_{110}$ direction closest to the wire axis rotates towards it leading to the typical fibre texture. A particular case arises, when the initial lattice orientation of a grain is such that no $h_{110}$ direction is preferred. This occurs when the $h_{100}$ direction is parallel to the wire axis. In this case, four of the $h_{110}$ directions form an angle of $45^\circ$ with the wire axis and the remaining two form an angle of $90^\circ$. This behavior can be seen in pole Fig. 3 (c). The lattice of this grain does not rotate towards the wire axis. It seems just to rotate due to the activity of the neighboring grains.

4.2. Grain curling in a 2D model

The 2D unit cell represents the elongated grain microstructure present after the first drawing steps. It consists of one layer of 3D cubic elements with their upper and lower faces constrained to remain flat, so that the model is in fact 2D. This approximation is plausible since simulations performed without these constraints show negligible deformation in the direction perpendicular to the plane. The outplane deformation is namely related to the lattice rotation of the grains towards the wire axis resulting in the $(110)$ fibre texture.

As the $(110)$ fibre texture is developed in the early drawing steps, the initial lattice orientation of all grains in the
2D model was prescribed as follows. The [101] direction of all grains is parallel to the wire axis, (see Fig. 4(a)). The only difference between lattice orientations of particular grains is the rotation of the lattice around the wire axis, as indicated by angle \( \phi \) in Fig. 4(b). The rotation angle \( \phi \) is given randomly, see Fig. 5(a) where the [10\( \bar{1} \)] direction is marked as \( \beta \).

Fig. 5 shows how these grains deform under equibiaxial compression. During the deformation process each individual grain deforms in an anisotropic manner. It remains nearly uncompressed in the [10\( \bar{1} \)] direction (denoted as \( \beta \)) and gets compressed preferentially in the [010] direction (perpendicular to \( \beta \)). For instance, grain I has its \( \beta \) direction in vertical position. Following its deformation history (see Fig. 6), we observe how the grain compresses in the direction perpendicular to \( \beta \) and it stays uncompressed in \( \beta \) direction. In order to accommodate the same deformation process of the neighboring grains II and III, the upper (lower) part of grain I is pushed to the right (left) and curling starts. Analogue deformation behavior can be observed for the remaining grains. The simulations show that the originally equiaxed grains do not deform axial symmetrically in the cross section but by plane strain which confirms the statement of Hosford [3].

In one of the very first attempts to describe the curling effect by means of crystal plasticity Hosford [3] stated that the stress to produce axial symmetric flow of individual grains was a factor 3/2 higher than the one required for producing plane strain flow. His conclusion was that individual grains prefer to deform by plane strain elongation and that the extra slip required for bending (curling) is probably considerably lower than the difference between...
the slip requirements of axial symmetry and plane strain. Our results obtained with a more detailed model confirm the plane strain deformation mode and show that stresses on the microscopic level occur which activate slip resulting in bending.

Finally, one can have a closer look at the activity of various slip systems. The simulations confirm dominant activity of those slip systems which have a high Schmid factor computed for equibiaxial compression. In this case, the Schmid factor is given by

\[ sf^{(s)}_{\text{eqb}} = m^{(s)}_i (a_i a_j + b_i b_j) s_j^{(s)}, \]

where \( a_i \) and \( b_i \) are orthogonal unit vectors in the direction of compression, both perpendicular to the wire axis. The slip systems with the highest Schmid factor (>0.4) are written bold in Table 1. Those slip systems are oriented in such a way that when they are active they contribute to elongation of the grains in axial direction, compression in direction [010], but no deformation in \( b \) direction. Furthermore, additional simulations assuming the activation of a single slip system family (first, second or third) lead to the same deformation shape as presented in Figs. 5 and 6. One can conclude that this anisotropic deformation of the individual grains along with the global interaction of the grains with their neighbors is the cause for curling and creates this particular microstructure.

5. Summary and conclusions

Taking into account the crystal orientation and the kinematics of crystallographic slip is essential to capture and describe texture evolution and curling. Therefore we developed a microstructural model which is based on a cubic unit cell representing the grain structure and the single crystal plasticity as material law. Successful predictions of the fibre texture evolution and curling are presented in this paper.

The employed approach allows to capture details such as grain interaction and it can be extended to analyze grain crack initiation and boundary separation, which are the current issue of our interest. An appropriate hardening model and realistic parameters will be necessary for quantitative studies. Improvements of the FEM model like adaptive meshing and smooth meshing of grain boundaries are further tasks.

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