Macromechanical finite-element simulations for predicting microstructures by experimental calibration

T Mehner¹, A Bauer², B Awiszus² and T Lampke¹

¹Institute of Materials Science and Engineering, Chemnitz University of Technology, 09125 Chemnitz, Germany
²Professorship Virtual Production Engineering, Institute for Machine Tools and Production Processes, Chemnitz University of Technology, 09107 Chemnitz, Germany

E-Mail: thomas.mehner@mb.tu-chemnitz.de

Abstract. Macromechanical simulations provide excellent opportunities for rapid calculations of forming processes. Geometrical dimensions and residual stresses can be calculated with very good agreement. More complex forming simulations (e.g. crystal dynamic simulations or calculations with representative volume elements) are necessary if microstructural magnitudes, like crystallite sizes and microstrains, have to be included. Using the example of cold-rolling, this paper aims to describe a different approach for connecting macromechanical finite-element simulations with key parameters of the microstructure. By means of X-ray diffraction and confocal microscopy, crystallite sizes, microstrains, texture and roughness values are determined and correlated to the plastic strain. The plastic strain can be simulated easily and the microstructure after forming can be predicted. As a result of this calibration, more complex simulations can be avoided. Nonetheless, these calibrated macromechanical simulations can be used for the estimation of microstructure-related properties, like the corrosion behaviour.

1. Introduction

The macromechanical finite-element analysis (FEA) is a versatile tool for the simulation of forming processes. Especially, fast simulations of large volumes can be performed and geometrical measures, plastic strains and residual stresses can be simulated with good accordance after performing a proper calibration of the simulation [1–2]. In these studies, it was found that the mesh with the associated remeshing parameters as well as the friction model and friction parameters are of great importance concerning this calibration [3].

However, physically relevant magnitudes, like crystallite sizes, microstrains, roughnesses or textures are not an outcome of these simulations. Thus, more complex forming simulations (e.g. crystal dynamic simulations or calculations with representative volume elements (RVE)) are necessary to include them. Hereby, RVE were connected to the laws of crystal plasticity where the deformation mostly takes place, because of dislocations in the lattice structure. Different models provide various mechanisms to implement hardening effects, material damage, diffusion processes or recrystallization [4–7]. Therefore, RVE are often used for modelling of more complex material behaviour with the related micromechanical effects while using reinforced composites [8-10] or dual phase steels [11-12].

In this paper, a different approach is presented using experimental calibration curves: Exemplified by cold-rolling, for different plastic strains (and different rolling-pass sequences), crystallite sizes, microstrains, roughnesses and textures calibration curves are determined experimentally and fitted by proper functions to be correlated to the FEA simulations. For proving the accuracy of the results,
rolling-pass sequences that were not used for calibration are simulated and compared with the experimental values.

2. Materials and methods
For the experimental cold flat rolling, a commercial DC04 sheet was cut into samples by water-jet cutting with initial measurements of 100 mm × 40 mm × 2 mm and a composition of 0.042 % C, 0.242 % Mn, 0.035 % Al, 0.011 % Si, 0.013 % S, 0.010 % P (mass fraction). The rolling was performed on a Duo/Quarto EW 105x100 strip rolling mill (Bühler und Co GmbH) with a roll speed of 12.12 rpm and different rolling-pass sequences (Table 1) and plastic strains. After rolling, the width of all samples was reduced to 14 mm by water-jet cutting to receive a homogenous sample state. Each sample was taken from the centre of the sheet with a distance of 13 mm from the edges.

Table 1. Rolling-pass sequences used.

| Final sheet thickness (mm) | Rolling passes, sheet thickness (mm) |
|---------------------------|-------------------------------------|
| 2.0                       | none                                |
| 1.8                       | 2.0–1.8                             |
| 1.7                       | 2.0–1.7                             |
| 1.5                       | 2.0–1.7–1.5                         |
| 1.5                       | 2.0–1.5                             |
| 1.3                       | 2.0–1.7–1.5–1.3                     |
| 1.3                       | 2.0–1.5–1.3                         |
| 1.1                       | 2.0–1.5–1.3–1.1                     |
| 0.9                       | 2.0–1.5–1.3–1.1–0.9                 |
| 0.7                       | 2.0–1.5–1.3–1.1–0.9–0.7             |
| 0.5                       | 2.0–1.5–1.3–1.1–0.9–0.7–0.5         |

FEA simulations were performed employing the tool simufact.forming 13.0 with a simulation setup as shown in figure 1. The sample geometry as well as the rolling parameters (size of the rolls, rolling kinematics) are identical with the real process. Furthermore, the numerical calculation was processed as 3D coupled setup with a temperature of 20 °C for workpieces, tools and environment. The friction was determined over a combined friction model (Coulomb and shear friction) with μ = 0.15 and m = 0.3. The mesh of the specimen was generated from hexahedral elements with 0.5 mm edge length and 4 elements over the sheet thickness. Therefore, the remeshing parameter was set to start the remeshing at an element deformation of 40 %. The material data for the used DC04 were generated experimentally by flat compression tests (at room temperature with a strain rate of 0.1 s⁻¹) and the calculated values were implemented into the simulation via data table. The plastic strains were determined by averaging over at least 50 nodes in the centre of the sample.

X-ray analyses were performed at the surface of the samples at positions in their centre along the rolling direction. X-ray crystallite sizes and microstrains of the samples were determined by X-ray diffraction (XRD) using a diffractometer D8 Discover (Bruker AXS) with Co Kα radiation (information depth of about 15 μm). The tube parameters were: 40 kV, 40 mA, point focus. For beam focussing and limiting, polycap optics and a 0.5 mm pinhole collimator were employed. The used 1D detector Lynxeye XE with 2.1° aperture angle allows measuring with effective measurement times of 192 s/step at a step width of the diffraction angle (2θ) of 0.01°. The 2θ range was 20°–127°. The evaluations of the line width were done with the programme TOPAS (Bruker AXS) under
consideration of device-related line-broadening effects. “Microstrain” denotes the FWHM(2θ) of the Gaussian part of the line profile divided by \( \tan \theta \) and is closely related to the dislocation density. Textures were measured utilising a diffractometer D5000 (Siemens) with Co K\(_\alpha\) radiation, 40 kV, 15 mA, point focus, a 1 mm pinhole collimator and a scintillation counter. Three pole figures of α-Fe, \{110\}, \{200\} and \{211\}, were measured at diffraction angles of 52.4°, 77.3° and 99.8°, respectively. Tilt angles of 0°–80° with step sizes of 5° for both rotation and tilt were used with a measurement time of 2 s/step. The evaluations were done with the programme MULTEX (Bruker AXS). At least four measurements were averaged for each XRD result.

The roughness average \( R_a \) was determined from measurements with a laser scanning microscope (LSM) VK-X200K (Keyence) with a magnification of 400x and an evaluated length of 4.8 mm. The cut-off wavelengths \( \lambda_s \) and \( \lambda_c \) were set to 2.5 µm and 800 µm, respectively – taking the standard DIN EN ISO 3274 into account. For each sample, 20 roughness profiles in the centre of the sample in rolling direction were evaluated and averaged.

Uncertainties given in the diagrams are confidence intervals with confidence levels of 95 %.

3. Results and discussions

The novel approach that will be used within this paper is based on the v. Mises equivalent plastic strain \( \varphi \) of the sample. It can be calculated by the individual plastic strains in the x, y and z directions:

\[
\varphi = \sqrt{\frac{2}{3} \left( \varphi_x^2 + \varphi_y^2 + \varphi_z^2 \right)}
\]  

(1)

Due to the special sample preparation, the plastic strain is almost homogeneously distributed across the entire sample (figure 2). Small deviation occur at the corners only. The FEA provides plastic strains for the samples, which are shown in figure 3.

Figure 1. Simulative setup of the cold flat-rolling process.

Figure 2. FEA simulation of the distribution of the plastic strain (sample 2.0 mm–1.7 mm–1.5 mm).
The FEA results indicate that the plastic strains are independent on the rolling-pass sequence if the final thickness is the same. Along the processing route 2.0–1.5–1.3–1.1–0.9–0.7–0.5, the plastic strain increases quadratically with the number of 0.2 mm thickness-reduction steps.

In the following, the correlation between the plastic strain of the samples and their structural properties is shown. The surface roughness is an important parameter in many applications; it will affect e.g. the corrosion behaviour, friction or sealing properties. $R_a$ is expected to decrease with progressive rolling.

![Figure 3. Plastic strains for the considered samples, calculated by FEA.](image)

In figure 4, the measured values of $R_a$ are shown, depending on the plastic strain. The fitting function used is an exponential decay that provides $(0.312 \pm 0.009) \text{ } \mu m$ as the asymptotical value of $R_a$. Due to the decay constant of the fitting function $(0.102 \pm 0.013)$, an almost constant roughness is reached for plastic strains above 0.4. Therefore, after the rolling pass 2.0–1.5 mm, $R_a$ is less than 0.02 $\mu m$ above the asymptotical value. The complete fitting function is expressed by:

$$R_a(\text{fit}) = 0.643 \text{ } \mu m \cdot \exp\left(\frac{-\varphi}{0.102}\right) + 0.312 \text{ } \mu m$$

In a similar way, the crystallite sizes and microstrains of the samples, measured by XRD, can be evaluated (figure 5). Exponential-decay fitting functions were used. The crystallite sizes show a strong decay with a decay constant of $0.105 \pm 0.014$ and an asymptotical value of $(106 \pm 3)$ nm. Thus, the decay constant is very close to the one of the $R_a$, which means that the relative decrease of these magnitudes due to cold rolling is very similar. However, it has to be pointed out that the crystallite size of the sheet with $\varphi = 0$ is larger than the maximum value XRD can determine (about 300 nm). Thus, this value (500 nm) is estimated only. Assuming larger values (2000 nm), the decay constant decreases to $0.049 \pm 0.009$ and the asymptotical value increases slightly to $(110 \pm 4)$ nm with $R^2 = 0.904$. Thus, significant differences $> 10 \%$ between the two fits occur for low plastic strains ($\varphi < 0.35$). However, the fit quality is better for the fit mentioned first, with the equation:
crystallite size (fit) = 390 nm \cdot \exp \left( \frac{-\varphi}{0.105} \right) + 106 \text{ nm} \tag{3}

The experimental microstrains show an almost constant value for plastic strains above 0.2. The exponential decay follows the equation:

\text{microstrain (fit)} = -0.141^\circ \cdot \exp \left( \frac{-\varphi}{0.086} \right) + 0.221^\circ. \tag{4}

Thus, the microstrain reaches a maximum value of 0.221° even for large plastic strains; i.e. above \( \varphi \approx 0.4 \), the dislocation density is constant.

Figure 4. Measured roughness average values dependent on the calculated plastic strains with an exponential decay fitting function (\( R^2 = 0.928 \)).

Figure 5. Crystallite sizes and microstrains for the samples with exponential-decay fitting functions (\( R^2 = 0.921 \) and 0.938, respectively).
The texture can hardly be expressed with one single number. Depending on the application in which the product will be used, different magnitudes may be of interest. In this paper, the fraction of the texture component with \{200\} lattice planes parallel to the surface is evaluated. Due to the cold rolling of DC04, there are two more texture components: \{211\} and \{111\} lattice planes parallel to the surface. In addition, there is an isotropic fraction that declines with progressive rolling passes. The initial state (2.0 mm sheet) was hot rolled, but this kind of rolling texture can still be measured. However, about 40\% of the measured intensity in the pole figures is isotropic for these sheets. In figure 6, the pole figures of a 2.0–1.5 mm sheet are shown.

\textbf{Figure 6.} Pole figures (stereographic projection with arbitrary intensity scale) of a cold-rolled 2.0–1.5 mm DC04 sheet, \{110\} (left), \{200\} (centre) and \{211\} (right). RD indicates the rolling direction.

For all of the measured cold-rolled sheets, the most dominant texture component is the \{111\} component. Its fraction is about 38\% for the 2.0 mm sheet and only increases to about 46\% for the 0.5 mm sheet and thus is hardly affected by cold rolling. A stronger influence is found for the \{200\} component and the isotropic fraction, figure 7.

\textbf{Figure 7.} Fraction of the \{200\} texture component as well as the isotropic fraction for the samples with exponential-decay fitting functions.
For low plastic strains, the isotropic fraction is decreasing quickly. Thus, an exponential fitting function with two decay constants is used. The $\{200\}$ component can be described by:

$$\text{fraction } \{200\} \text{ (fit)} = -14.9\% \cdot \exp \left(-\frac{\varphi}{0.26}\right) + 18.8\%.$$  

(5)

Using the equations (2)–(5), the structural properties can be predicted. To prove the validity, the values of two additional sheets with different rolling pass sequences are compared with the calculated ones. The rolling pass sequences in table 2 differ significantly from the ones used in the fitting process. Still, the results are in excellent agreement with differences clearly below the experimental uncertainties.

**Table 2.** Comparison of calculated and measured values.

|                              | 2.0–1.4–1.2 mm | 2.0–1.9–1.4–0.8 mm |
|------------------------------|----------------|-------------------|
| Plastic strain               | 0.65           | 1.12              |
| Roughness average (µm)       |                |                   |
| experimental/calculated      | 0.300 ± 0.021/0.313 | 0.293 ± 0.021/0.312 |
| difference                   | 0.013 (4.3 %)  | 0.019 (6.5 %)     |
| Crystallite size (nm)        |                |                   |
| experimental/calculated      | 106 ± 9/106    | 105 ± 11/106      |
| difference                   | ≈ 0 (< 0.1 %)  | 1 (1.0 %)         |
| Microstrain (°)              |                |                   |
| experimental/calculated      | 0.23 ± 0.04/0.22 | 0.228 ± 0.024/0.221 |
| difference                   | -0.01 (4.3 %)  | -0.007 (3.1 %)    |
| Fraction $\{200\}$ texture component (%) | | |
| experimental/calculated      | 17.6 ± 1.6/17.8 | 18.5 ± 0.3/18.6   |
| difference                   | 0.2 (1.1 %)    | 0.1 (0.5 %)       |

4. Summary and conclusions

It has been shown that the structural properties average roughness, crystallite size, microstrain and texture can be clearly correlated with the plastic strain, which can be calculated by the FEA with low deviations. For the used DC04 cold-rolling process (with $\varphi = 0$ for the hot-rolled sheet with 2 mm thickness), the relations in table 3 were determined. The independence of these properties is most probably a consequence of the low strain-rate sensitivity of the material. If this sensitivity is high, such relations may not be applicable.

Macromechanical FEA simulations allow calculations of plastic strain $\varphi$ and residual stresses. When including the relations in table 3 into the FEA, it allows predicting of the above-mentioned structural properties, which are not a direct outcome of the simulations. Furthermore, with these calculated magnitudes, it is possible to deduce additional material’s behaviour, e.g. corrosion properties. Thus, the usefulness of the FEA can be enhanced significantly without additional calculation time needed.
Table 3. Fitting parameters based on the equation \( y(\phi) = A \cdot \exp(-k/\phi) + y_0 \).

| Property                      | \( A \)       | \( k \)       | \( y_0 \)       |
|-------------------------------|---------------|---------------|---------------|
| Roughness average (\( \mu m \)) | 0.643 \( \mu m \) | 0.102         | 0.312 \( \mu m \) |
| Crystallite size (nm)         | 360 nm        | 0.109         | 105 nm        |
| Microstrain (\( ^\circ \))    | -0.141\(^\circ\) | 0.086         | 0.221\(^\circ\) |
| Fraction \{200\} texture component (%) | -14.9 %      | 0.26          | 18.8 %        |

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