Crystal Plasticity Model Validation by Single-Grain Indentation Tests

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Abstract
In this paper the experimental and numerical results of a spherical indentation test applied to a single grain of a rolled steel sheet is presented. In addition to measuring the indentation load-displacement curve, ex situ, micron resolution, 3D x-ray microscopy measurements of the local lattice rotations in the indented material are performed. Simulations of this test have been done by means of 3D finite element calculations using a crystal plasticity material model which has been previously adjusted to polycrystalline shear and tensile tests. It is shown that the load-displacement curves and the lattice rotations are well predicted by the calculations. As an example of these results a comparison of the measured and calculated lattice rotations is shown. Although the rotation magnitude is slightly overestimated, the spatial distribution of the rotation field is well predicted. Due to results like this a validation of the crystal plasticity model on the microscopic grain scale has been achieved. An additional sensitivity study revealed that the friction between indenter and grain affects the lattice rotations below the indentation up to a depth of five times the indentation depth.

Keywords: Material characterization, Identification and validation, Crystal plasticity, Lattice rotations

Introduction

Crystal plasticity models are of increasing importance for scientific and industrial purposes. However, one of the biggest problems in the application of these models remains their identification and validation (Cailletaud et al. 2003). Especially for the characterization of the plastic properties of rolled sheets, large efforts have been undertaken to find proper experimental techniques (Kuwabara 2007). The classical way to adjust the parameters of a crystal plasticity model is to use experimental results of tests with polycrystalline specimens. In addition to this classical method, the use of experimental data obtained from single grain (polycrystalline embedded) experiments has been suggested. In particular, small size indentation tests are well documented. Nevertheless, load-displacement curves obtained from such tests often do not contain sufficient information to identify all material parameters, so a sustainable identification is not possible. However, additional information about the behaviour of materials can be obtained from measurements of deformation fields, such as lattice rotations in the indented material. In this paper a combination of a model identification on the macroscopic (polycrystalline) scale and a validation on the microscopic (single crystalline) scale is presented.

Material

All specimens have been taken from a rolled DC04 steel sheet with a thickness of 0.8 mm. In the initial condition the material showed an average grain size of 16 µm. In order to achieve single-crystalline behaviour it is necessary that the indentation is sufficiently distant from grain boundaries. This condition causes problems because of the low grain size of the DC04, however sufficiently large grain sizes of ~100 µm (**Fig. 1**) were achieved after annealing the sheet for 18 hr at 1200° C and subsequent furnace cooling.

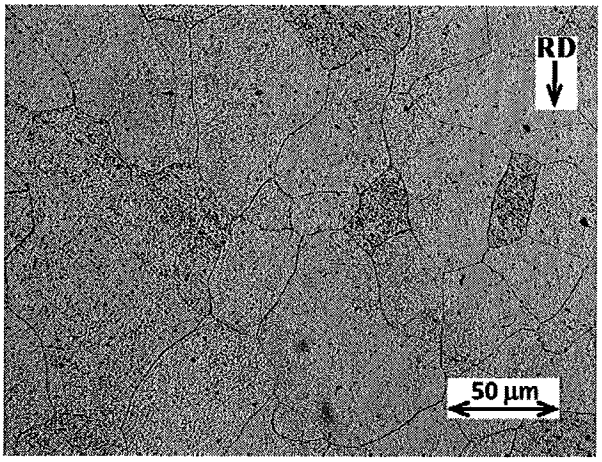

Figure 1. Micrograph of the heat treated DC04 steel.

Experiments

In addition to measuring the indentation load-displacement curves, ex situ 3D x-ray microscopy on the Sector 34 ID-E microbeam facility at the Advanced Photon Source at Argonne National Laboratory was used to make micron resolution measurements of the local lattice orientations resulting from 500 mN force (100 µm radius sapphire tip) spherical indentations. The 3D x-ray microscopy measurements were performed as described previously (Yang et al. 2004) using a 0.5 µm diameter polychromatic microbeam and an area detector providing angular orientation determinations with ~0.01 degree angular precision. The rotational deformation measurements were made on a plane perpendicular to the sample surface passing through the middle of the indentation by sequential line scan

measurements (to depths of 40 µm below the sample surface) with one micron translations of the sample between scans.

Numerical Model

Material model. The material behaviour is described by a standard crystal plasticity model (Bertram 2008). Non-Schmid effects have been neglected in the current context, and crystallographic slip on the {110}<111> and {112}<111> slip systems is assumed. The stresses are calculated by an anisotropic linear elastic law, and the viscous ansatz of Hutchinson (1976) is used to calculate the shear-rates

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \operatorname{sgn}\left(\frac{\tau_\alpha}{\tau_c}\right)\left|\frac{\tau_\alpha}{\tau_c}\right|^{\frac{1}{m}}. \quad (1)$$

Herein $\dot{\gamma}_0$ and m are material parameters and τ_c is the critical resolved shear stress, which is assumed to be the same for all slip systems. The evolution of the critical resolved shear stress is described by a Kocks-type hardening law

$$\tau_c = \tau_{c0} + (\tau_s - \tau_{c0})\left(1 - \exp\left(\frac{-\theta_0 \gamma}{\tau_s}\right)\right) + \theta_\infty \gamma \quad (2)$$

wherein the critical resolved shear-stress depends exclusively on the accumulated shear

$$\gamma = \int \sum_\alpha \dot{\gamma}_\alpha dt \quad (3)$$

of all slip systems α. The four material parameters in Equation (2) are the initial critical resolved shear stress τ_{c0}, the saturation stress τ_s, the initial hardening modulus θ_0, and the remaining hardening modulus θ_∞. This model has been implemented in a user subroutine (UMAT) of the finite element code ABAQUS. The discretization is done by means of a backward Euler scheme (Böhlke 2006).

Parameter identification. The hardening parameters have been adjusted to polycrystalline shear tests performed by Bouvier et al. (2006). All other parameters have been defined previously. A detailed description of the model identification procedure is given by Hoffmann et al. (2010a) and Hoffmann (2011).

Table 1. Predefined and identified material parameters.

parameters of the	$\dot{\gamma}_0 = 10^{-3}\ s^{-1}$
viscose approach	$m = 0.02$

elastic constants	$K_{1111} = 207$ GPa
	$K_{1122} = 121$ GPa
	$K_{1212} = 105$ GPa

hardening	$\tau_{c0} = 57.5$ MPa
parameters	$\tau_s = 115$ MPa
	$\theta_0 = 802$ MPa
	$\theta_\infty = 42.4$ MPa

3D finite element model. The micro-indentation test has been simulated by a 3D finite element calculation using an FE-model which is subdivided into separate parts for the specimen and the indenter. By neglecting the influence of the surrounding grains, the whole specimen is modelled as a single-crystal, which has the same orientation as the particular indented grain (**Table 2**).

Table 2. The orientation of the indented grain with respect to the sample coordinate system (see **Fig. 2**).

direction of the sample coordinate system	crystallographic direction in (hkl)
X	(3.71, -1.00, 2.86)
Y	(-1.00, 3.49, 2.52)
Z	(-1.05, -1.02, 1.00)

In **Fig. 2** the complete specimen mesh, which consists of 22000 linear selectively reduced integrated hexahedral elements (B-bar elements) is shown. Boundary conditions of zero displacement at the bottom and stress free conditions on the sides have been applied. The influence of these conditions on the misorientations has been investigated and found negligible. The indenter is modelled as a rigid sphere, and the contact interaction between indenter and specimen is implemented by standard Abaqus algorithms. Hard contact and Coulomb friction have been assumed in normal and tangential direction, respectively. Due to the fact that the material behaviour is modelled by crystal plasticity, the indentation simulation determines the orientation changes at every calculation point of the specimen. These orientation changes can be compared directly to those measured by the microbeam X-ray method. It is convenient to divide the orientation changes into the three rotations around the axes of the sample coordinate system (**Fig. 2**). This has been performed by a vector decomposition of the Rodrigues-vector. For material parameters in the simulations, we used those listed in **Table 1**.

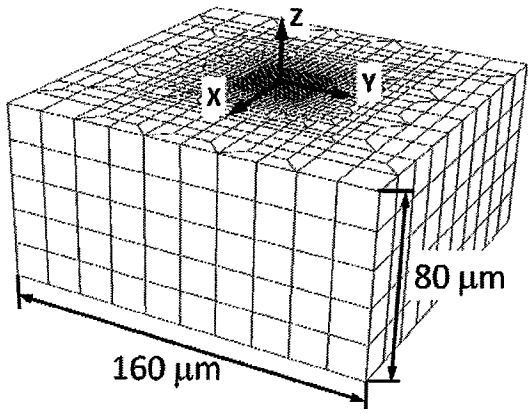

Figure 2. FE-mesh of the specimen and sample coordinate system.

Results and Discussion

Fig. 3 shows that the measured and calculated load-displacement curves are in good agreement, but for several reasons this should be interpreted with caution. One important fact is that the hardening parameters of the constitutive model are adjusted to the non-annealed material.

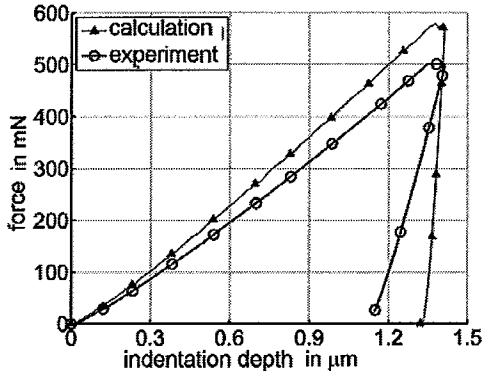

Figure 3. Measured and calculated load-displacement curve.

Therefore the calculated load-displacement curve behaves too stiffly along the loading path. Furthermore, the hardening parameters depend on the homogenisation method used in the identification scheme. Within this work the Taylor model has been used to simulate the polycrystalline tests and this will lead to lower hardening parameters than the use of a representative volume element. We note that the measured lattice rotations in **Fig. 4** are reproduced in detail by the calculation. In particular the spatial distribution is nicely captured. However, the magnitude of lattice rotation overestimated by the model. This has been also observed by Zaafarani et al. (2008) for a fcc and by Britton et al. (2010) for a hcp material.

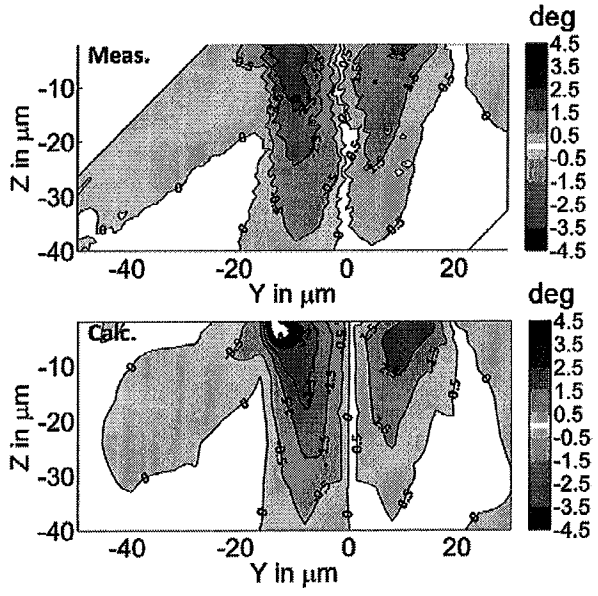

Figure 4. Comparison of the measured and calculated lattice rotations around X.

The prediction of higher lattice rotations corresponds to the difference between the measured and calculated load-displacement curve during unloading. As shown in **Fig. 3** the calculation overestimates the remaining indentation depth. Whether this is because of a possible plastic backflow or by the compliance of the testing device has not be clarified at this point. By taking into consideration that the material model has been adjusted to polycrystalline tests, the prediction of the micro indentation test is in good agreement with the experimental findings. Therefore a validation of the material model on the single crystalline micro scale has been achieved. We note that in **Fig. 4** rotations are normal to the plane of the measurements only (i.e. in-plane). Unlike the case for sharp indenters (Britton 2010), the symmetry associated with the central slice of spherical indentations results in out-of-plane rotations much smaller than the in-plane rotations and although of interest, they are second order compared to the in-plane rotations and outside the scope of this paper. We comment further that we do not believe that the free surface boundary conditions at 80 µm are responsible for the prediction of larger rotations than measured because the discrepancies are large only in the central region immediately under the indenter. Similar arguments make it unlikely that the proximity of other grain orientations is responsible for the prediction of larger rotations below the 100 µm radius indenter, which wets the sample surface with a diameter of only 25-30 µm.

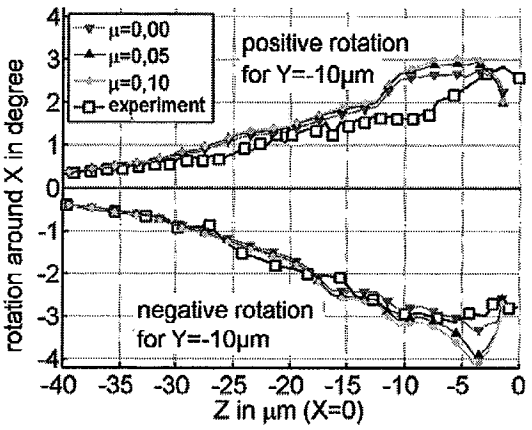

Figure 5. Influence of the friction coefficient on the calculated lattice rotations.

It is still an open question as to how lattice rotation data can be used to identify material parameters on the micro scale. An important step toward answering this question is the investigation of the sensitivity of lattice rotations to various parameters. In **Fig. 5** the influence of the friction coefficient on the lattice rotations is shown. The results are evaluated along two vertical lines, which extend from the crystal surface (Z=0 µm) to a point deep inside the crystal (Z=-40 µm). It can be seen that below a depth of approximately 5 times the indentations depth the lattice rotations

are hardly affected by the friction between the indenter and the specimen.

Conclusion

A sustainable validation of a crystal plasticity model on the single crystalline scale has been achieved. Since the identification of the material model has been performed by the use of polycrystalline tests, an indirect link between the macroscopic and microscopic material behaviour has been found.

Acknowledgement

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