A numerical approach to evaluate roughness effects on localization and damage in sheet materials

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Abstract. In dualphase steels damage initiation can be triggered by interface debonding between ferrite and ferrite or ferrite and martensite, by martensite breaking, or by strain localization in the ferritic matrix. The roughness of sheet materials strongly influences the damage initiation and accumulation of dualphase steel, because roughness provokes local strain concentrations which accelerate the evolution of ductile damage. The presented study quantifies the effect of surface roughness on strain localization and ductile damage evolution in a numerical simulation framework established on different scales. On the macro-scale, an uncoupled phenomenological ductile damage mechanics model is applied to ductile material failure. On the microscale, sub-models are investigated that contain information on surface roughness profiles. Two different conditions are investigated: i.) samples that have been only grinded, ii.) samples that have been grinded and polished. In both cases, the surface roughness is characterized by white light confocal microscopy, and the raw data of these experimental measurements are used as input data for a numerical algorithm that reproduces surfaces with the same statistical roughness profiles. The numerical studies reveal the pronounced influence of surface roughness on material resistance against ductile failure.

1. Introduction
When the automotive industry started to consider aluminium alloys for car body structures to fulfil lightweight engineering requirements about three decades ago, steel producers were motivated to develop a new class of sheet materials with high strength, excellent cold formability and high crashworthiness. The materials development resulted in the “1st generation of advanced high strength steels” (1G AHSS), which are typically processed into a multiphase microstructure by thermal or thermo-mechanical treatments. Typical examples for steels from 1G AHSS are dualphase (DP) steels. Their microstructure is composed of a ferritic matrix with dispersed martensitic islands. Due to this special microstructure composition, DP steels show an inhomogeneous strain distribution when subjected to any kind of mechanical loads [1].

Conventional car body steels were typically evaluated based on their strain hardening property and cold formability, whereas damage initiation and accumulation were not seriously assessed when component design options were discussed. This was justified by the simple observation that damage initiation and subsequent damage accumulation were only triggered after significant amount of necking. Engineers therefore concluded that the guiding principle for component design should be to avoid any strain localization. Consequently, necking criteria for sheet materials were developed, and experimental procedures to characterize the onset of necking during sheet metal forming were applied. Probably, the most widely used criterion is the forming limit diagram (FLD) [2], which however provides reasonable estimations of the material’s formability only for proportional strain paths. Improved predictions under
non-proportional strain paths could be achieved with the forming limit stress diagram, which evaluates principal stresses in the sheet plane instead of plastic strains [3].

With the development of the second generation of AHSS (2G AHSS), formability prediction was challenged by the simple fact that cracks could appear prior to necking under certain stress states [4]. Consequently, neither the FLD nor the FLSD were able to give reasonable estimations of the cold formability. This paved the way for new approaches to characterize the cold formability of sheet materials. Since for materials of 2G AHSS damage and fracture set the limits for cold formability instead of necking phenomena, damage mechanics approaches were prepared.

The failure behaviour of sheet materials from 2G AHSS is generally ductile, with void nucleation, growth and coalescence as underlying mechanisms. Porous plasticity models typically offer void evolution equations, and they consider the actual void volume fraction in their yield potentials in order to capture the damage-induced softening effect. The most widely used porous plasticity model is most probably the GTN model, which was initiated by Gurson [5] and further developed by Tvergaard and Needleman [6-8]. Modifications of the original GTN model [9-11] became necessary because its applicability is restricted to loading situations characterized by sufficiently high stress triaxiality, which is not always given in sheet materials.

In contrast to coupled models that consider the damage-induced softening effect, uncoupled approaches do not take into account any influence of ductile damage on the plastic reaction of a material [12]. Instead, criteria are presented that characterize failure of the corresponding material point. These criteria are regularly expressed as limit strains that depend on the local state of stress. For isotropic materials, the latter one is expressed by stress triaxiality and the normalized Lode angle. These two parameters are derived from the invariants of the stress tensor and the deviatoric stress tensor, respectively.

In the past, damage mechanics models were successfully applied to predict failure of samples and components made from sheet steels of 2G AHSS. However, with the continuously increasing complexity of formed parts in industrial practise, and the continuous materials development, failure cases could be observed that seemed to depend on surface roughness influences. But even though it seems to be logical that extensive roughness leads to plastic strain peaks and therefore promotes the underlying mechanisms of ductile damage, quantitative approaches with a high predictive capability have not yet been presented. In this paper, an approach is therefore suggested that has got the potential to assess and quantitatively predict the surface roughness sensitivity of ductile damage in DP steels. The approach is established on two different scales. On the macroscopic scale, simulations are carried out with an uncoupled approach which makes use of the von Mises plasticity model combined with a stress state dependent, strain based ductile fracture criterion. These failure strains are defined as functions of stress triaxiality and normalized Lode angle. Noteworthy, this model definition is achieved by employing the user-defined VUMAT subroutine of the modified Bai-Wierzbicki (MBW) model [13-15] with a special adjustment of some of the model parameters.

On the microscopic scale, sub-models are investigated. They are connected to the macroscopic simulations via weak macro-micro-coupling, meaning to perform macroscopic simulations first to determine deformation boundary conditions for the following microscopic simulations. The sub-models, however, contain information on surface roughness properties. These data are experimentally revealed by scans with a light-optical confocal microscope. The surface roughness values are statistically evaluated and considered when the microstructure model is generated. Likewise, numerical stress analysis can be carried out to study whether sufficiently high strains for ductile failure result from the roughness-induced inhomogeneous strain distribution.

In this paper, the procedure is demonstrated for samples made from steel grade DP1000. However, the samples have undergone two different treatments to manipulate surface roughness conditions. In one case, samples were practically polished, whereas in the other one, samples were grinded. Both experimental and numerical studies reveal rather pronounced roughness influences on the material’s mechanical performance, which is characterized in simple sheet metal bending tests.
3. Material
A steel of grade DP1000 was selected for the presented investigations. The material properties are briefly summarized in the following paragraphs.

|        | C   | Si  | Mn  | P   | Cr  | Mo  | Ni  | Cu  | Nss |
|--------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| DP1000 | 0.07| 0.30| 2.55| 0.008| 0.68| 0.12| 0.03| 0.11| <0.0001 |

The material’s chemical composition is presented in table 1. Similar to many other DP steels, the material has got a comparably slim alloying concept with less than 0.15 % of C and a little less than 3 % of Mn.

In order to reveal strength and ductility properties, quasi-static isothermal tensile tests were conducted at room temperature. With the material’s yield stress of 770 MPa and its ultimate tensile stress of 983 MPa, the pronounced strain hardening properties are proven. The uniform elongation and $A_0$ fracture strain are 5.2 % and 11.0%, respectively. Since the experimental results covered only a comparably small region of strain, inverse FEA analysis was carried out to find a suitable description of the material’s flow behaviour at larger strains. As presented in figure 1, this analysis resulted in the following approximation of the flow curve:

$$\sigma_{\text{yld}} = 0.5 \cdot 1300(2.3e^{-14} + \varepsilon^p)^{0.075} + 0.5 \cdot [266.2 + 507.1(1 - e^{-73.942\varepsilon^p})].$$

Figure 1. Different flow curve extrapolations

4. Macroscopic model
For the numerical simulations, an uncoupled simulation framework was applied which combines a von Mises plasticity model with a strain based ductile fracture criterion. Since ductile fracture is well-known
to be stress state dependent, one can rely on the stress triaxiality and the Lode angle to assess the damage and failure behaviour of isotropic materials. With the principal stresses denoted by $\sigma_1$, $\sigma_2$ and $\sigma_3$, the three invariants of the stress tensor are defined respectively by

$$ p = -\sigma_m = -\frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3). $$

$$ q = \sigma_e = \frac{1}{2\sqrt{3}}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]. $$

$$ r = \frac{27}{2}(\sigma_1 - \sigma_m)(\sigma_2 - \sigma_m)(\sigma_3 - \sigma_m)^{\frac{1}{3}}. $$

Using these invariants, stress triaxiality and Lode angle can be calculated according to

$$ \eta = -\frac{p}{q}, $$

$$ \theta = \frac{1}{3}\arccos\left(\frac{q}{r}\right). $$

While the influence of stress triaxiality on ductile fracture has been extensively described in literature [17-22], the consideration of the Lode angle is relatively new for plasticity and ductile fracture models [23-25]. For symmetry reasons, the Lode angle is defined for $0 \leq \theta \leq \pi/3$. By normalizing the Lode angle, the Lode angle parameter or normalized Lode angle is expressed by

$$ \bar{\theta} = 1 - \frac{6\theta}{\pi}. $$

The so-called ductile fracture locus (DFL) defines the instant of ductile fracture in the selected approach. It defines the equivalent plastic strain to ductile fracture as a function of the stress triaxiality and the normalized Lode angle:

$$ \bar{\varepsilon} = \left(c_1 \cdot \exp(-c_2 \cdot \eta) - c_3 \cdot \exp(-c_4 \cdot \eta)\right)\bar{\theta}^3 + c_5 \cdot \exp(-c_6 \cdot \eta) $$

![Figure 3: Ductile fracture locus of steel DP1000.](image)
5. Simulation framework to evaluate roughness effects on ductile failure properties

Rectangular samples with a length of 60 mm, a width of 20 mm and a thickness of 1.5 mm (initial thickness) were produced from the investigated steel DP1000. These samples were manufactured to be tested in bending experiments, but before these experiments were conducted, all samples received treatments to adjust the surface roughness. Half of the samples were grinded with 80-grit sand paper, whereas the other half was practically grinded with finest sand paper followed by polishing with grain size of 1 μm. After this surface treatment, the adjusted roughness profiles were experimentally investigated by white light confocal microscopy. Figure 4 exemplarily shows the typical differences between the two configurations. Obviously, remarkable roughness differences are revealed by these experimental campaigns. The experimental data were afterwards processed by filtering out the high-wavelength component of the surface profiles using Gaussian filter with cut-off wavelength at 80 μm. The remaining components of each configuration were quantified as surface roughness depth distribution functions as presented in figure 5.

The surface roughness information was afterwards used to construct sub-models for numerical simulations that contain surface roughness information. In this procedure, points are randomly placed on the top surface of each sub-model corresponding to its depth distribution function. These points are then connected to each other by using a polynomial function. Figure 6 exemplarily shows two different geometrical sub-models which represent the investigated roughness levels. The significant differences between the two surfaces become evident.
At the current stage, the sub-models are defined for a homogeneous material which is again described by the von Mises plasticity model. However, the effect of crystallographic orientations could be investigated in case that crystal plasticity models are used to describe the plastic material reactions. In such case, grains would have to be reproduced in the microstructure model, and their crystallographic orientation would have to be assigned. This work is planned for the near future, where the microstructure shall be reconstructed by using the multiplicatively weighted Voronoi tessellation technique. However, currently these effects have not yet been considered.

3-point-bending tests were performed on all samples according to the testing procedure VDA238-100. The geometrical set-up is presented in figure 7. The roller diameter D equalled 18 mm, and the roller distance was 6 mm. The punch had a radius of 0.5 mm. All experiments were conducted until the sample started to extensively slip along the rollers, so that almost no more increase in local equivalent plastic strain below the punch could be expected. This behaviour was observed for punch displacements of approximately 12 mm. Afterwards, macroscopic numerical simulations with the presented model were performed. These simulations served to determine displacement boundary conditions to be applied on the different sub-models presented above. Figure 8 shows the distribution of equivalent plastic strain in the bending sample, indicating the strong strain localization on the bottom side of the sample in the position below the punch. Therefore, the sub-models were connected to the centre point of the sample on the bottom side.

Figure 9 shows a comparison of the punch force-displacement curves from experiment and macroscopic simulation. During the experiments, extensive slipping of the sample began at a punch displacement of 12 mm. At that instant, cracks were already obvious in the samples with the higher roughness, whereas the smoother samples were free from any defects that could be detected with a human being’s naked eye. This already indicates the pronounced effect of surface quality on ductile damage evolution. In addition, it also sets the requirements for the simulation framework, which has to prove its capability to reproduce these experimental findings.

![Figure 7. Geometrical set-up of 3-point-bending tests.](image)

![Figure 8. Distribution of equivalent plastic strain in the bending sample (Mesh size: 0.1 mm).](image)

![Figure 9. Left: Comparison between force-displacement curves between simulation and experiment at different surface configurations. Middle: surface of fine grinded and polished sample. Right: surface of 80-grit sand paper grinded.](image)
The sub-models were simulated with the displacement boundary conditions that were identified in the macroscopic simulations. It implies that a weak macro-micro-coupling was applied to connect macroscopic and microscopic simulations.

Figure 10. Distribution of equivalent plastic strain in the sub-models (mesh size of 0.1 µm) for the critical punch displacement of 12 mm. Left: fine grinded and polished, right: 80-grit sand paper grinded.

Figure 10 shows the distribution of equivalent plastic strain in the two different sub-models for the critical punch displacement of 12 mm. Obviously, there is a pronounced strain localization in the sample with the high roughness, whereas the strains remain much more moderate in the smoother surface configuration. However, the surface roughness also alters the local state of stress. In order to decide whether the strain concentration is sufficient to provoke ductile failure, the calculated maximum equivalent plastic strains have to be normalized towards the ductile failure strains for the present stress triaxiality and normalized Lode angle. Figure 11 therefore presents a summary of the exploitation of the ductile failure strains. It shows a value of 76 % for the smooth surface after grinding and polishing (no fracture), but a value of 216 % (fracture) for the 80-grit sample. From these values one can conclude that the simulation reproduces the experimental finding that the smooth sample does not show fracture events in the bending test, whereas the rough sample fails.

Figure 11. Exploitation of the ductile failure strain. Left: fine grinded and polished, right: 80-grit sand paper grinded.

6. Conclusions

- Surface roughness strongly influences ductile damage and failure in the investigated steel of grade DP1000.
- The pronounced influence is based on the inhomogeneous strain distribution that results from the geometrical micro notches.
- By applying a sub-model simulation framework, the plastic strain inhomogeneity can be quantified, so that also failure predictions can be given.
- Future studies should aim to refine the microscopic simulations. Especially in DP steels, the microstructure morphology strongly influences the plastic strain distribution due to the pronounced mechanical property mismatch between ferrite and martensite. It can be expected that more precise sub-modelling with crystal plasticity models and statistically representative microstructure models should be able to significantly improve the predictive capability of the simulation framework.
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