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# Plasticity and failure behavior modeling of high-strength steels under various strain rates and temperatures: microstructure to components

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#### **Abstract**

The aim of this study is to establish an integrated material modelling approach, micro, macro and component scales, for investigating the plasticity, damage and fracture behaviour of modern high-strength steels under various strain rates and temperatures. With the established relations between different scales, the approach ultimately provides a knowledge-based and efficient alternative for the damage-tolerant microstructure design to the conventional empirical rules. In this study, we will present the models working at different scales and the scaling strategy between them. For a more general application than quasistatic and room temperature, the models are formulated with strain rate and temperature dependency. All models are calibrated by experiments on the corresponding scale and also validated by experiments not involved in the calibration procedure or tests from a higher length scale. As the ultimate goal of the approach is to guide the microstructure design, a fine-resolution digital representation of the microstructure is targeted in the study. In addition to the standard phase fraction, grain size and shape features, fine-tuning of the microstructural features, such as texture and misorientation distribution is also implemented into the synthetic microstructure model. The impact of these individual microstructure features and their combination on the macroscopic and component level performance is studied and the optimized microstructure for the desired improvement of the mechanical property can be identified by the proposed approach.

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#### 1. Introduction

Integrated computational materials engineering (ICME) has been intensively developed for the recent decade driven by the product and process optimisation and new material development (Butz et al., 2010; Helm et al., 2011). This study employees the ICME principle to explore its potential in the field of ductile damage and fracture particularly under high strain rates. An integrated multiscale modelling approach is established to seamlessly link models working at different length scales and eventually to guide the design of the microstructure for steels with improved damage tolerance.

The crashworthiness is a structural level measure of component properties that matters significantly for the automotive industry. It is normally characterised by crash box tests in case of axial loading, involving large plastic deformation and ductile damage/fracture behaviour under high strain rates and complicated loading history. Therefore, instead of the conventional "microstructure-mechanical property relationship", the study brings the scope one level up to the structure scale. The general methodological flow of the study is illustrated in Fig. 1. It starts at 12 o'clock position on the characterisation of the structural crashworthiness property. The bridging of the performance indicator with the mechanical property profiles is conducted by macroscopic modelling. For the linking between the microstructure and the mechanical properties, the representative volume element (RVE) model is employed allowing consideration of the microstructure parameters and at the same time bridging the equivalent quantities from microstructure to macroscopic level by incorporating a crystal plasticity material model. Furthermore, the processing parameters are connected to the microstructure via the processing models. With the established modelling approach, the optimal microstructure can be identified and, in addition, the optimised processing parameters will also be calibrated and applied to production for the validation of the entire approach in both lab and component scales. In the current study, only the macroscopic and microscopic modelling are considered.

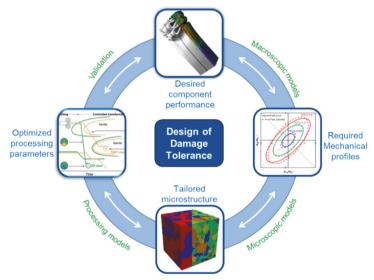


Fig. 1. The methodological flow of the multiscale study on the high-strength steel sheets for the crashworthiness property across the component level, lab level, microstructure and process routines.

#### 2. Multiscale Modelling

## 2.1. Macroscale modelling - MBW damage model

By taking the advantages of both uncoupled models and coupled models (Besson, 2009), Lian et al. (2013) proposed a hybrid damage mechanics model that combines a phenomenological criterion for damage initiation related to the microstructure-level degradation of materials, and a continuum damage mechanics (CDM) based damage

evolution law for progressive damage accumulation till final fracture. The damage initiation criterion relies on the Bai-Wierzbicki (BW) uncoupled damage model (Bai and Wierzbicki, 2008), thus it is also referred to as the modified BW (MBW) model (Lian et al., 2015). With this modelling approach, the multiscale characterisation of both damage and fracture can be realized. As the damage initiation is related to the microstructure of materials, the damage initiation locus and its stress-state dependency can be up-scaled from the mesoscale simulations accounting for the microstructural inhomogeneity (Lian et al., 2014). Recently, the model was extended to account for cleavage fracture (He et al., 2017) and damage development under non-proportional loading conditions (Wu et al., 2017). The concept of the model formulation is illustrated in Fig. 2. The detailed equations are not listed due to the space limit.

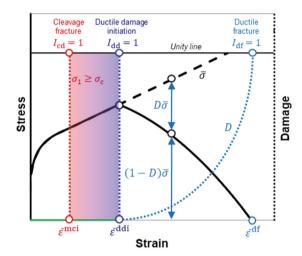


Fig. 2. Schematic illustration of the modified Bai-Wierzbicki (MBW2018) damage model for cleavage and ductile fracture.

## 2.2. Micro and mesoscale modelling – Crystal plasticity model

On the micro and mesoscale, crystal plasticity model is employed to describe the micro-deformation mechanism and correlate the microstructure with mechanical behaviour. Crystal plasticity models have been intensively developed and applied to simulating the material behaviour of single crystal or polycrystal, taking the crystallographic orientations of grains into account (Roters et al., 2010; Tikhovskiy et al., 2008; Wang et al., 2004). Based on metallographic analysis of microstructure, mesoscale simulations of statistically-characterised and microstructure-based polycrystal are performed by using the method of virtual laboratory. In the current study, complex deformation mechanisms, e.g. nonplanar spreading of the screw dislocation cores, are not taken into account and the dislocation slip is only assumed to occur in the 24 main slip systems resulted from slip family {110}<111> and {112}<111>.

## 3. Materials and Experiments

In this study, a dual-phase steel (DP1000), which is often used for the crash box component in an automobile is investigated. The steel sheet with a thickness of 1.5 mm is composed of ferrite and martensite phases and the phase fraction of martensite is about 50%. Additionally, the average grain size for both ferrite and martensite is less than  $2 \mu m$ .

An extensive experimental program (Fig. 3) is designed involving various sample geometries that cover a wide range of stress states and tests are performed under quasi-static and high strain rate conditions up to 2500 s-1 and from room temperature to 300°C to obtain the plasticity and fracture description of the material. In addition to the lab experiments, the crash box is tested under axial loading in a drop weight device. The energy to be dissipated by the profile can be adjusted by the weight and the height of the drop hammer. With respect to the designed profile geometry with the sheet thickness of 1.5 mm and to the high strength dual-phase steel, the applied energy is around 10 kJ with a drop mass of 129.5 kg and a drop height of 8 m.

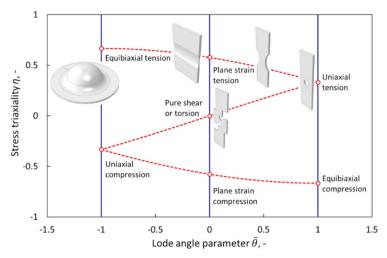


Fig. 3. Experimental program of lab tests and their characteristic stress states in the space of stress triaxiality and Lode angle parameter (Lian et al., 2013).

#### 4. Results and Discussion

## 3.1. Macroscopic level

The lab experiments under different strain rates and temperatures are used to calibrate the material parameters of the MBW model for both plasticity and damage/fracture parts. It is noted that the flow curves for high strain rates are carefully treated: instead of using the adiabatic flow curves directly, an elaborate procedure is performed to convert the adiabatic flow curves to isothermal ones and the Taylor-Quinney coefficients are also calibrated for different strain rates. The calibrated model is then used to simulate the structure-level crash box test.

The results comparisons between experiments and simulation are shown in Fig. 4. Generally, compared to the experiments, the recurrence of crash box material behaviour including the force-displacement response, total impact energy absorption, and globe deformed shape is accurately obtained in the simulation. In terms of the deviation on the energy/force-displacement curves, the current material parameter set results in a harder material behaviour in the simulation. The reason can be related to the mesh mismatch between the lab test simulation and the crash box simulation. Therefore, a non-local formulation of the damage model is being developed to overcome the mesh influence and allow more accurate prediction on the structure level. Referring to the local deformation and damage/fracture development, the crack initiation and propagation within the foldings of the crash box specimen is also well captured by simulation.

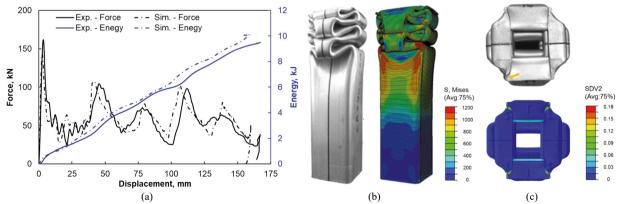


Fig. 4. Crash box test: (a) Experiment and numerical comparison of the force/energy-displacement curves of the test; (b) Deformed sample and finite simulation result after impact – stress contour; (c) Comparison of the cracks on deformed sample and FE simulation result after impact – damage contour.

## 3.2. Micro and mesoscopic level

In the microstructure model, various features, such as phase fraction, the distributions of grain size, grain shape, crystallographic orientation and misorientation are considered, as shown in Fig. 5. The resolution for both phases is down to grain level.

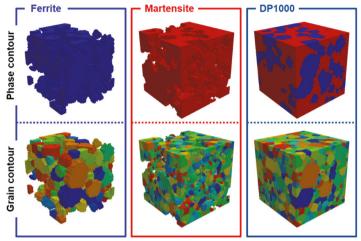


Fig. 5. Visualization of the DP1000 RVE (upper row for phase maps and lower row for grain maps).

The material parameters for the crystal plasticity model is calibrated based on nanoindentation tests on single grains. The upscaling of the microscopic model to macroscale is powered by the virtual experiments. In Fig. 6, the result of a simple uniaxial tension test on the RVE is shown. It is clear that the numerical flow curve fits well to the experiment one. From the deformation and stress contour, it is clear to reveal the stress partitioning between two phases as well as different grains.

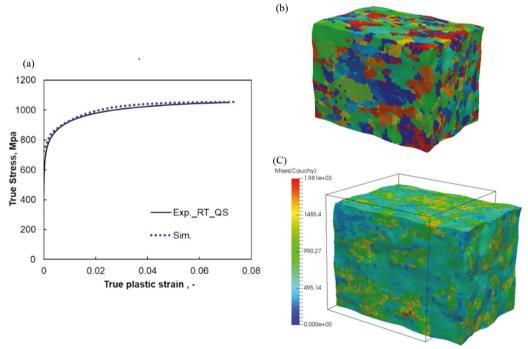


Fig. 6. (a) Flow curve comparison between the experiments and the RVE simulation; (b) The deformation of the RVE with its grain map; (c) The stress contour of the deformed RVE.

#### 5. Conclusions and Outlook

The study illustrates the establishment and application of a multiscale modelling approach in the field of ductile fracture under very high strain rates and complex loading history. Based on multiscale verifications of the approach, the study contributes to the in-depth understanding between microstructure and crashworthiness for steel sheets and the derivation of new design rules for modern damage-tolerant high-strength steels. The outlook of the study is to further extend the modelling approach to connect the microstructure with processing parameters.

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