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Dependency of the Young's modulus to plastic strain in DP steels: a consequence of heterogeneity ?

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Abstract

The accurate springback prediction of dual phase (DP) steels has been reported as a major challenge. It was demonstrated that this was due to the lack of understanding of their nonlinear unloading behavior and especially the dependency of their unloading moduli on the plastic prestrain. *A so-called compartmentalized finite element model was developed.* An improved compartmentalized finite element model was developed. In this model, each element was assigned a unique linear elastic J2 plastic behavior without hardening.

15 The model's *specificity* novelty lied in the fact that:

- i) a statistical distribution was discretized in a deterministic way and used to assign yield stresses to structures called compartments,
- ii) those compartments were randomly associated with the elements through a random compartment element mapping (CEM).

20 Multiple CEM were simulated in parallel to investigate the intrinsic randomness of the model. The model was confronted with experimental data extracted from the literature and it was demonstrated that the model was able to reproduce the dependence of the apparent moduli on the tensile prestrain. It was also observed that the evolution of the apparent moduli was predicted

even if it was not an explicit input of the experimental dataset used to identify the input parameters of the model. It was then deduced that the shape of the hardening and the *dependancy*dependency of moduli on the prestrain were two manifestations of a single cause: the heterogeneous yield stress in
5 DP steels.

Keywords: Dual phase steels, Apparent modulus, Young's modulus evaluation, Heterogeneity, Springback.

1. Introduction

Dual phase (DP) steels exhibit an outstanding combination of strength and
10 ductility. They are widely used in the automotive industry where they contribute to the vehicle mass reduction and thus to greater fuel efficiency (Tasan et al., 2015). This being said, the complexity of their mechanical behavior is especially high and many scientific challenges have to be addressed before they can be used with full background knowledge. Among those, the accurate
15 prediction of springback is one of the greatest (Wagoner et al., 2013). It is known that the apparent Young's modulus of most metallic alloys is influenced by an applied prestrain (Yoshida et al., 2002; Pham et al., 2015) and that this is especially true in the case of DP steels. It has also been demonstrated that this phenomenon affects the ability to predict springback (Eg-
20 gertsen and Mattiasson, 2010; Yu, 2009; ul Hassan et al., 2016). While the *dependence*dependency of the apparent modulus to the prestrain is observed by many researchers, the mechanisms at stake are not yet fully determined. Therefore, several ways have been followed to take this evolution of the apparent modulus into account. The most widely used and arguably the most

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successful is the phenomenological modeling developed in numerous papers (Yoshida and Uemori, 2003; Kim et al., 2013; Sun and Wagoner, 2011; Lee et al., 2013; Ghaei and Taherizadeh, 2015; Xue et al., 2016; Zajkani and Hajbarati, 2017; Torkabadi et al., 2018). These studies do not focus on the
5 underlying causes of the phenomenon but only aim to reproduce it, in most cases by using the model proposed by Yoshida et al. (2002). The drawback of phenomenological methods is that they rely on a fine-tuning stage of an ever-increasing number of parameters.

In parallel, other methods have been aiming at establishing a relation be-
10 tween the material's physical properties and its macroscopic behavior. As pointed out by Paul (2013), the intrinsic dual phase heterogeneity of DP steels triggers strain incompatibility between the soft ferrite phase and the harder martensite phase. Several two-phase models have been developed using local phenomenological models as well as crystal plasticity to take into account the
15 bimodal mechanical behaviors (Kadkhodapour et al., 2011; Ramazani et al., 2012; Moeini et al., 2017). Random microstructures have also been used with relative success (Furushima et al., 2009, 2013a,b; Ayatollahi et al., 2016; Khan and Gautham, 2018). Still, this global simulation process has been un-
able to reproduce correctly the non-linear unloading behavior of DP steels and
20 so it has been failing to determine the quantitative changes in the apparent modulus unless finally using the phenomenological Yoshida-Uemori model.

As stated by Tasan et al. (2015), the causes of heterogeneity in DP steels are multiple: on the one hand, heterogeneous dislocation microstructure, grain size distribution, presence of impurities and on the other hand, strong
25 differentiation between the mechanical behaviors of its constituent phases which are themselves randomly distributed in the material. Then, a third

way has been explored to deal with these observations. It relies on introducing heterogeneity in the model in a more generalized way using a statistical spatial distribution of yield stresses (Tabourot et al., 2012, 2013). This compartmentalized model has shown that it can reproduce experimental observations with fewer adjustable parameters than phenomenological models and that their predictions are more realistic (Bizet et al., 2017).

In this paper, an improved version of the compartmentalized model was used to simulate and analyze the apparent modulus of DP steels. Section 2 is dedicated to the description of the compartmentalized model. Then, the model is applied to retrieve experimental data extracted from the literature. In section 3, the predictions of the model are discussed and confronted with the other existing modeling paradigms.

2. The compartmentalized model

A compartmentalized model is a random heterogeneous finite element model in which the material properties of every element arise from those of a substructure called a compartment. Each compartment has unique material properties. In the presented model each element is a compartment. Compartments are not designed to represent a specific physical structure or scale such as grains. Their only purpose is to introduce a controlled amount of heterogeneity in the model to produce specific effects on the macroscopic mechanical behavior. The implementation of the compartmentalized model described in this section is made available by the authors (python libraries : Compmo2 (Charleux and Roux, 2019b) and Argiope (Charleux et al., 2019), full code example : Compmo2 Documentation (Charleux and Roux, 2019a))

2.1. Mesh and boundary conditions

In this paper, the finite element simulations were carried out using the commercial implicit solver Abaqus/Standard (2018 version). Fig. 1 represents the cubic Representative Volume Element (RVE) test sample. The initial dimensions of the RVE were $l \times l \times l$ along $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$ where $l = 1$. Only intensive properties such as stress and strains were extracted from the model. Consequently, the problem was dimensionless and the value of l had no impact on the results. ~~A structured $10 \times 10 \times 10$ hexahedric mesh was used.~~ A structured $10 \times 10 \times 10$ hexahedric mesh was used. Periodic boundary conditions were applied in a similar way to (Wu et al., 2014). The sample was loaded in tension and the true tensile stress σ as well and true tensile strain ε were calculated.

2.2. Compartmentalized material definition

In a compartmentalized model, the material properties are distributed randomly among the elements of the mesh. This procedure has been greatly improved compared to the intuitive one used by the authors in previous articles (Tabourot et al., 2012, 2013, 2014; Bizet et al., 2017). This legacy procedure is described in Fig. 2 while the new one is represented in Fig. 3.

Each compartment is associated with a unique but very basic, isotropic, linear elastic and J2 perfectly plastic material. Consequently, no hardening is implemented in any of those materials.

Moreover, the elastic behavior of all compartments is homogeneous. Their Young modulus has a fixed value $E = 213$ GPa and their Poisson's ratio is $\nu = 0.3$. These values are in agreement with Chen et al. (2016a).

2.3. Yield stress distribution

The yield stresses σ_y are distributed among the compartments following a statistical distribution noted DIST. It is defined by its probability density function (PDF) noted $f(\sigma_y)$ and its cumulative density function (CDF) noted $F(\sigma_y)$. In this case, the distribution is the weighted sum of two Weibull sub-distributions with PDFs $f_1(\sigma_y)$ and $f_2(\sigma_y)$ that verify:

$$f(\sigma_y) = w_1 f_1(\sigma_y) + (1 - w_1) f_2(\sigma_y) \quad (1)$$

And:

$$f_i(\sigma_y) = \frac{k_i}{\lambda_i} \left(\frac{\sigma_y}{\lambda_i} \right)^{k_i-1} \exp \left(- \left(\frac{\sigma_y}{\lambda_i} \right)^{k_i} \right) \quad (2)$$

Where:

- k_i and λ_i are respectively the shape parameters and the scale parameters of the Weibull sub-distributions,
- w_1 is the weighting factor between each sub-distribution and it verifies $w_1 \in]0, 1[$.

The five input parameters $P = \{k_1, k_2, \lambda_1, \lambda_2, w_1\}$ fully define the plastic behavior of the RVE. The values of the yield stresses associated with each compartment could then be calculated using a Random Number Generator (RNG) associated with the PDF defined above. However, this solution would mean that for a given value of P , multiple different sets of yield stress values could be possible because of the random nature of the RNG. As a consequence, the model would not be deterministic and most optimization scheme to identify the parameters would be compromised. To overcome this issue, a procedure

has been developed to discretize the distribution in a deterministic way as described in Fig. 4.

1. The model contains N compartments, each occupying an equal part of the whole model volume. As a consequence, each compartment C_i is assumed to represent a cumulative probability of $1/N$. The CDF is equally split along the vertical axis in N parts separated by $N + 1$ thresholds values noted F_t , where $F_{t_0} = 0$ and $F_{t_N} = 1$.
2. The CDF is inverted using the Brent zero finding algorithm (Brent, 1973) implemented in the Python library Scipy (Jones et al., 2001), $N + 1$ threshold yield stress values σ_t are determined. This process is described in Fig. 4-a.
3. Each individual compartment then represents a unique portion of the distribution. Since only a single value of $\sigma_{y,i}$ has to be associated with each compartment C_i , the mean value of distribution on the interval $[\sigma_{t,i}, \sigma_{t,i+1}]$ is chosen:

$$\sigma_{y,i} = \frac{\int_{\sigma_{t,i}}^{\sigma_{t,i+1}} \sigma f(\sigma) d\sigma}{\int_{\sigma_{t,i}}^{\sigma_{t,i+1}} f(\sigma) d\sigma} \quad (3)$$

2.4. The Compartment Element Mapping

Each element E_j is associated with a compartment C_i by a discrete bijective mapping function referred to as the Compartment Element Mapping (CEM) as presented in Fig. 5. The CEM is initialized by shuffling the $\{1, \dots, N\}$ list, creating the required association between the compartments and the elements. The CEM is the only source of the randomness of the model and thus it is the way to control it. As a consequence, as long as the CEM is not reinitialized,

the model response to a given set of input parameters P is deterministic. In this paper, a set of 10 random CEMs was generated by random shuffling and was used all along.

2.5. Input parameter identification on a single loading-unloading-reloading cycle

The true tensile stress vs. true tensile strain curve of a DP980 steel was extracted from Fig. 2 in Ghaei et al. (2015) and is referred to as the experimental curve. This curve was separated into multiple loading, unloading and reloading cycles (MUR). The resulting data-set was split into two subsets represented in Fig. 6. The first subset noted **EXP-A** contains a monotonic loading up to 8% of strain and the last unloading-reloading cycle (LUR). It is essential to note that the evolution of the elastic moduli with the accumulated plastic strain cannot be observed on this subset because it contains only one unloading-reloading cycle. The second subset noted **EXP-B** contains the remaining experimental data.

For any given set of input parameters P and for each CEM c , a true tensile stress response can be simulated following the strain path of the test **EXP-A**. *Because the strain values of experimental and simulated curves are not coincident an interpolation is needed.* As experimental and simulated data are not interpolated on the same grid, it is necessary to interpolate them. The simulated stresses are therefore linearly interpolated on the strain value of the experimental curve **EXP-A**. The interpolated simulated stress is noted $\sigma_{ci}(P)$, where i denote each point of the **EXP-A** curve. The stress residuals vector $\delta\sigma_{ci}(P)$ between the calculated set of stresses and the experimental stress σ_{ei} is de-

defined as follows:

$$\delta\sigma_{ci}(P) = \sigma_{ci}(P) - \sigma_{ei} \quad (4)$$

The residual vector $\delta\sigma_{ci}(P)$ gathers the point to point stress residual for all CEMs at each measurement points.

The optimal input parameters P_{opt} were then calculated using the Levenberg-Marquardt least-square optimization algorithm (Levenberg, 1944) by minimizing the residual vector $\delta\sigma_{ci}(P)$.

With an educated guess of the starting point of the Levenberg-Marquardt algorithm, the convergence was achieved after 70 evaluations of the cost function and thus after 700 individual simulations. The optimal numerical values of P_{opt} are given in the Table 1.

This way to proceed allowed us to determine not only the mean stress value but also the dispersion of the solutions associated with the different CEMs at each strain value. The mean stress value as well as min/max values are represented on Fig. 7. The associated yield stress distribution is represented in Fig. 8. The compartments yield stresses statistics are detailed in the Table 2.

2.6. Moduli calculation on multiple loading-unloading-reloading cycles

A new set of 10 simulations were run using the optimized input parameter set P_{opt} . These new simulations included multiple unloading reloading cycles. It is important to note that these multiple unloading reloading cycles were not used in the parameters identification stage. These multiple cycle simulations aimed to calculate the moduli as a function of the prestrain ε_u to evaluate the capacity of the compartmentalized model. The obtained mean stress value as

well as min/max values are represented on Fig. 9, and are noted **SIM-MUR** .

The moduli E_1, E_2, E_3, E_4 and E_c were then calculated following the definitions proposed by Chen et al. (2016b) as represented on Fig. 10 using the stress vs. strain curve **SIM-MUR**.

5 **3. Results and discussion**

3.1. Overall performances of the compartmentalized model

The Fig. 7 demonstrates that the compartmentalized model can reproduce efficiently the experimental loading/unloading behavior of a DP steel (DP980 here). This is also true for other existing models such as the QPE
10 model (Sun and Wagoner, 2011). However, the compartmentalized model is more efficient as it only relies on a homogeneous linear elastic coupled to a J2 plastic criterion without hardening behavior and 5 additional parameters (Tab. 1) to describe the material. This specificity makes the compartmentalized model's parameters easier to identify than those of its phenomenological
15 counterparts. In this paper, only 70 optimization iterations (700 simulations) were needed to identify the parameters required to fit the **EXP-A** experimental sub-data-set.

3.2. Compartment statistics

The identified parameters P_{opt} solely describe the level of heterogeneity
20 of the local yield stresses. Fig. 8 gives an accurate description of the optimal yield stress distribution.

Compared to other alloys previously modeled using the compartmentalized model (Bizet et al., 2017), it appears that distinguishing feature of the DP980 steel behavior is due to its exceptional heterogeneity that leads to a

wide range of distributed yield stresses. In that respect, 3 compartment sets are defined in the Tab. 2, each of them producing a given effect or property.

The Soft to Hard compartments (SHC) constitute the main lobe of the distribution and represent a fraction of 80.5%. If this population has to be modeled alone, a single Rayleigh distribution could be used. The upper bound of the yield stress of SHC fixed at 3000 MPa because all the elements having higher yield stress *always* never exhibited plastic strain in any simulation. This also means that the local von Mises stress field can sometimes reach very high values close to 3 GPa.

The Elastic compartments (ELC) represent 12.3% of the compartments. They are key compartments to model the specificity of materials exhibiting hardening at large strains such as DP980. If all compartments would become plastic during loading, the hardening would saturate. Hence, to exhibit hardening even at $\varepsilon \approx 10\%$, a significant proportion of the compartments must always remain elastic.

The Ultra-Soft compartments (USC) represent 7.2% of the compartments. They exhibit very low yield stresses. They don't play a key role during loading but their existence is strongly connected with the Bauschinger effect observed during unloading and the hysteretic behavior associated with unloading-reloading cycles. Indeed, at the end of the loading step (Fig. 7, $\varepsilon \approx 8\%$ and $\sigma \approx 1200$ MPa), when the unloading starts, most of these compartments rapidly *getbecome* plastic in the compressive direction during the first 200 MPa of *the* unloading. Thus, these compartments dissipate energy and increase the curvature of the unloading stress vs. strain curve at the end of the unloading step. The

same phenomenon appears symmetrically during reloading.

3.3. Moduli evolution predicted by the compartmentalized model

Fig. 11 represents the experimental measurements extracted from Fig. 5 of Chen et al. (2016b) and the values extracted from SIM-MUR using the same protocol as described in Fig. 10. First it appears in Fig. 11 that the evolution of E_1 and E_3 are overestimated by the compartmentalized model. However, in their paper, Chen et al. (2016b) state that the observed decrease in E_1 and E_3 in their data is small and could be an artifact due to a lack of resolution. Secondly, it appears that of E_2 and E_4 are in very good agreement like the chord modulus E_c . The optimization of the input parameters leading to the values of P_{opt} was performed on the dataset EXP-A (see Fig. 6) in which the evolution of the moduli is not included since there is only one unloading-reloading cycle. Yet the evolution of the apparent moduli predicted by the SIM-MUR simulations using P_{opt} is in good agreement with the experiments. This means that the compartmentalized model is not only able to reproduce the evolution of the apparent moduli, while its intrinsic modulus E is unchanged. It also implies that the decreasing apparent moduli are a necessity given the data contained in the EXP-A dataset. Consequently, in the context of the compartmentalized model, the strain hardening but also of the evolution of the apparent moduli are just two consequences of a single cause: the heterogeneity of the material which is the most significant result of this study.

Fig. 11 represents the experimental measurements taken from Fig. 5 in Chen et al. (2016b) as well as the values obtained by SIM-MUR using the protocol described in Fig. 10. Fig. 11 shows that the evolution of E_1 and E_3 is overestimated by the compartmentalized model. However, in their paper,

Chen et al. (2016b) indicate that the decrease observed in their E_1 and E_3 measurements is small in the face of measurement uncertainties and could thus be an artifact related to a lack of resolution. In contrast, the variations of E_2 , E_4 and E_c calculated by the simulation **SIM-MUR** using P_{opt} are in very good agreement with the experimental data. This implies, on the one hand, that the compartmentalized model is capable of reproducing the moduli decrease with a constant intrinsic Young's modulus E . On the other hand, since the optimization of the input parameters P_{opt} is carried out with the **EXP-A** dataset, which contains only one loading/unloading/reloading cycle, it follows that, in the context of the compartmentalized model, the decay of the apparent moduli is related to the shape of this cycle. These results indicate that strain-hardening, as well as the evolution of apparent moduli, are only two manifestations of a single cause: the heterogeneity of the material. It also shows that the compartmentalized model allows a physically realistic representation of the mechanisms involved in the plastic deformation of DP steels.

4. Conclusion

In this work, the compartmentalized model has been proved to be a relevant way to model the behavior of DP steels. The model was improved by separating its intrinsic spatial heterogeneity and its randomness into two independent contributions driven respectively by the DDP and the CEM. It has been shown that this improvement allows the model to be deterministic and thus that its input parameters P could be easily optimized as long as the CEM is kept unchanged. Results obtained from model simulations have been confronted with experimental pieces of evidence found in the literature and it

has been demonstrated that:

1. it can reproduce the overall shape of the stress vs. strain curve of the DP980 steel without needing the use of the variable intrinsic Young's modulus.
- 5 2. the evolution of the apparent moduli with the level of prestrain is predicted spontaneously when the model is optimized to reproduce the experimental LUR cycle.

Consequently, it has been postulated that the evolution of the moduli with the level of prestrain is just a consequence of the level of heterogeneity of mechanical properties such as yield stresses. The double Weibull yield stress
10 distribution with perfect elastic-plastic behavior is sufficient to give a very good global strain hardening representation.

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Parameter	Value
k_1	1.64
k_2	3.17
l_1	4.16×10^{-3}
l_2	3.42×10^{-2}
w_1	8.67×10^{-1}

Table 1: The parameters P_{opt} resulting from the optimization for the compartmentalized model.

Label	$\sigma_{y,min}$	$\sigma_{y,max}$	$\bar{\sigma}_y$	N_c	Behavior
USC	0 MPa	200 MPa	123 MPa	72	Ultra Soft
SHC	200 MPa	3000 MPa	865 MPa	805	Soft to Hard
ELC	3000 MPa	$+\infty$	6790 MPa	123	Elastic

Table 2: *Statistics on the compartment yield stresses associated with the optimized solution P_{opt} .* Statistical yield stress distribution in the optimized solution P_{opt} .

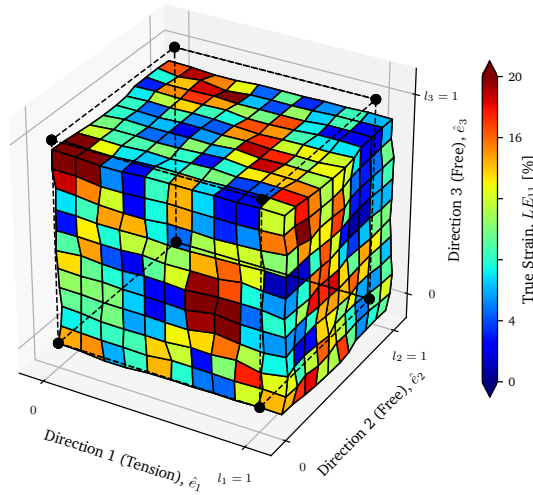


Figure 1: The RVE is represented in a deformed state under macroscopic tensile strain. The edges of the cubic RVE in its initial configuration are represented using dotted lines. The color map represents LE_{11} local logarithmic total strain along the tested direction. The heterogeneity of the strain field is visible and a shear band can be observed on the top face. The periodic boundary conditions are also visible as all opposite faces are identical modulo a translation.

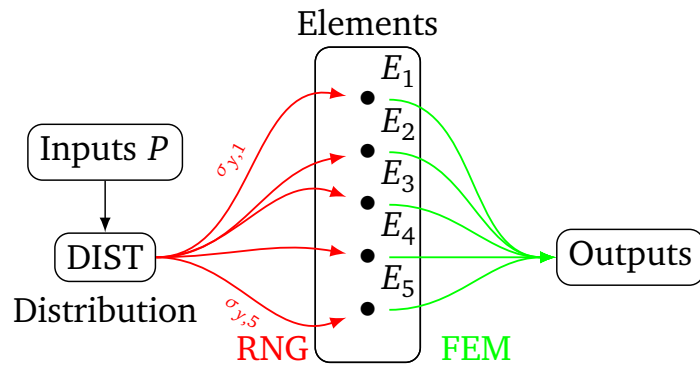


Figure 2: Schematic representation of the intuitive implementation of the compartmentalized model. The input parameters P are used to define the yield stress distribution DIST. A Random Number Generator (RNG) is used to calculate element yield stress $\sigma_{y,i}$ associated to each element E_i . The Finite Element Method is then used to solve the problem and generate outputs such as the tensile stress vs. tensile strain curve. The *relation link* between the input parameters and the output stress vs. strain curve is non-deterministic since two evaluations of the RNG with identical inputs lead to different outputs. Consequently, the optimization of the input parameters P cannot be done with classical optimization algorithms.

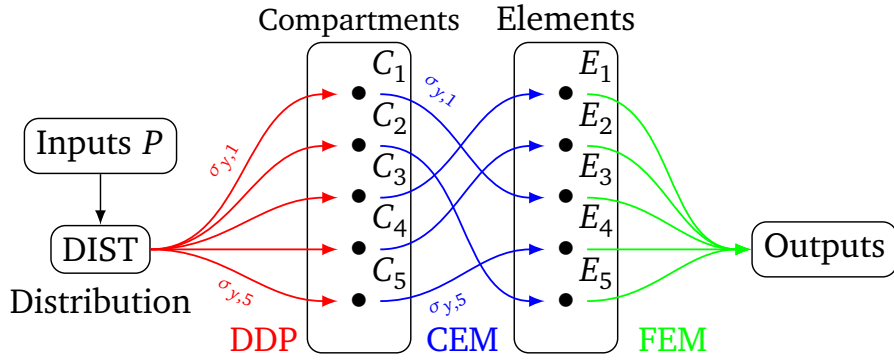


Figure 3: Schematic representation of the new approach developed in this paper. *Like in the intuitive approach, the input parameters P are used to define the yield stress distribution $DIST$.* As in previous approaches, the input parameters P are used to define the yield stress distribution $DIST$. Then, the distribution is discretized using the Distribution Discretization Procedure (DDP) described in Fig. 4 and N yield stress values $\sigma_{y,i}$ are calculated in the ascending order. Each of them is associated with a compartment C_i . Subsequently, the Compartment Element Mapping (CEM) is applied to associate each compartment C_i with a given element E_j . The CEM is initialized using a random draw algorithm. It can then be kept as *The CEM is initialized using a shuffling algorithm but it can be kept constant*, for example during the input parameters optimization process. As a consequence, the model is deterministic, and therefore the optimization of the input parameters P becomes possible with standard gradient-based algorithms such as Levenberg-Marquardt.

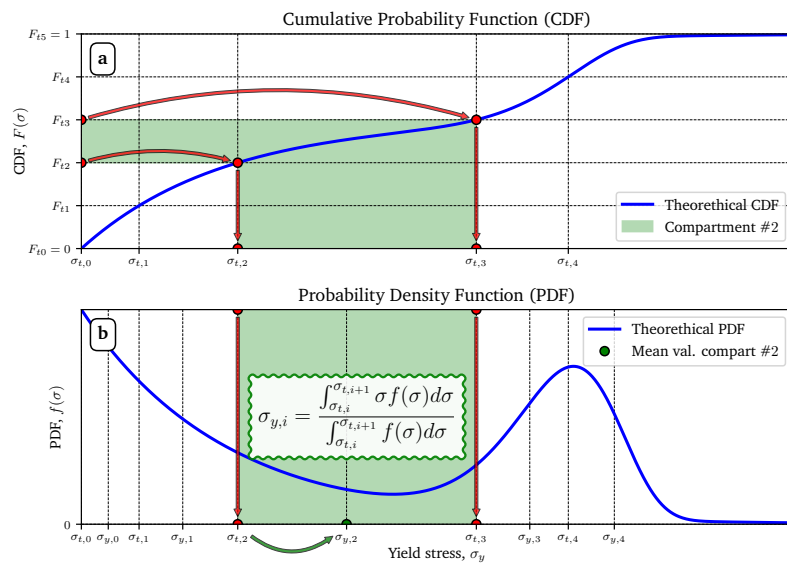


Figure 4: The Distribution Discretization Procedure (DDP): **(a)** The CDF is split vertically into N equal parts separated by $N + 1$ threshold values $F_{t,i}$. The CDF is *inversed reversed* and stress threshold values $\sigma_{t,i}$ are determined. **(b)** The yield stress values $\sigma_{y,i}$ are calculated as the average value of the distribution's PDF f over the $[\sigma_{t,i}, \sigma_{t,i+1}]$ interval.

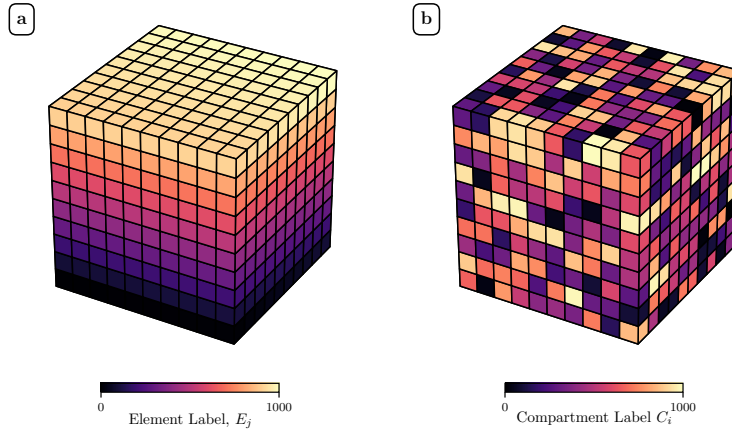


Figure 5: Graphical illustration of the Compartment Element Mapping (CEM). **(a)** The elements are labeled in a standard way. **(b)** Each compartment is associated with one element by a bijective mapping. Each CEM instance is created by shuffling the element labels. 10 different CEM are used in the paper, each of them being referred to as CEM-0, ..., CEM-9. Only CEM-0 is represented here.

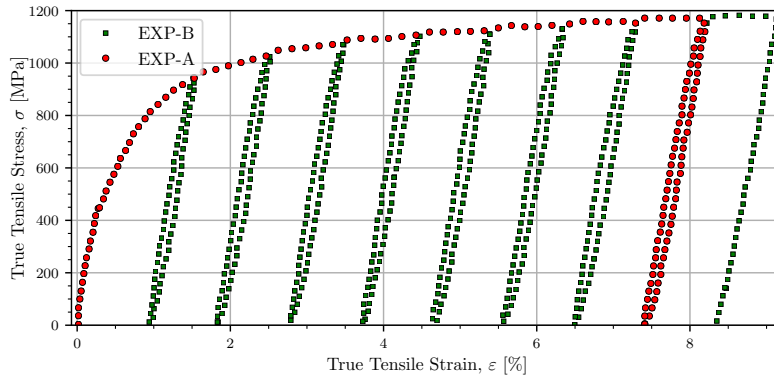


Figure 6: The experimental dataset noted EXP is extracted from Ghaei et al. (2015) and is composed of multiple loading, unloading and reloading steps. The dataset is split into two sub-datasets: EXP-A contains all the loading steps and the last unloading-reloading steps whereas EXP-B contains the remaining data.

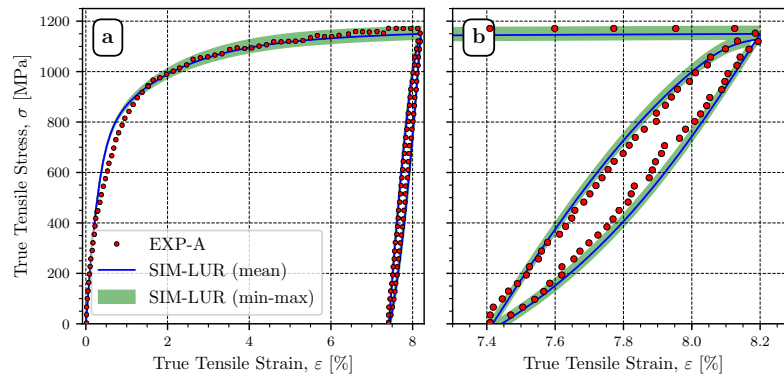


Figure 7: The compartmentalized model is optimized by fitting the output true tensile stress vs. true tensile strain to the experimental sub dataset EXP-A. (a) The whole curve is represented. (b) Zoom on the unloading-reloading step.

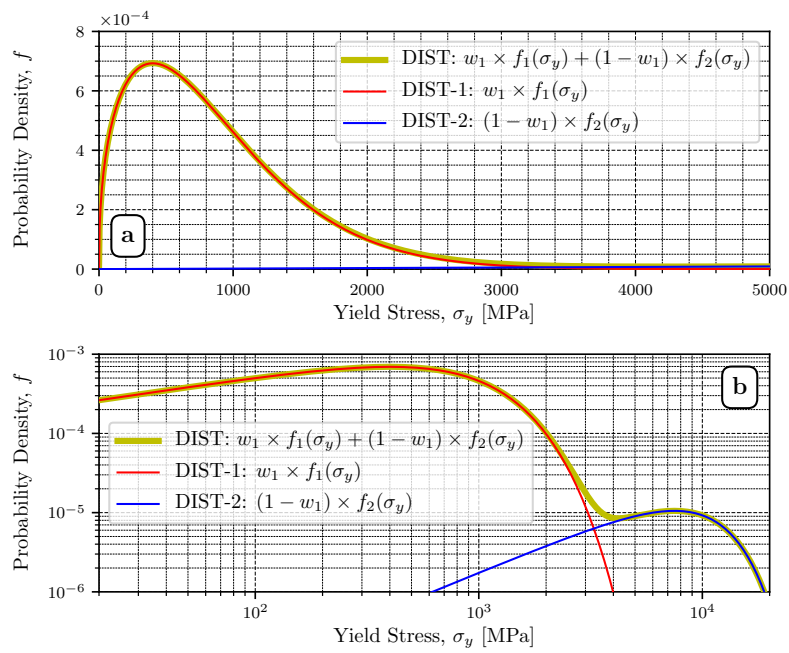


Figure 8: Representation of the statistical distribution of yield strength after optimization on the EXP-A dataset. *The statistical distribution of the yield stress values of the compartments after optimization on the EXP-A sub-dataset.* (a) linear scale representation. (b) log-log scale representation. The first Weibull distribution part DIST-1 is ~~en~~ represented in red, the second DIST-2 is represented in blue, the total distribution DIST is represented in yellow.

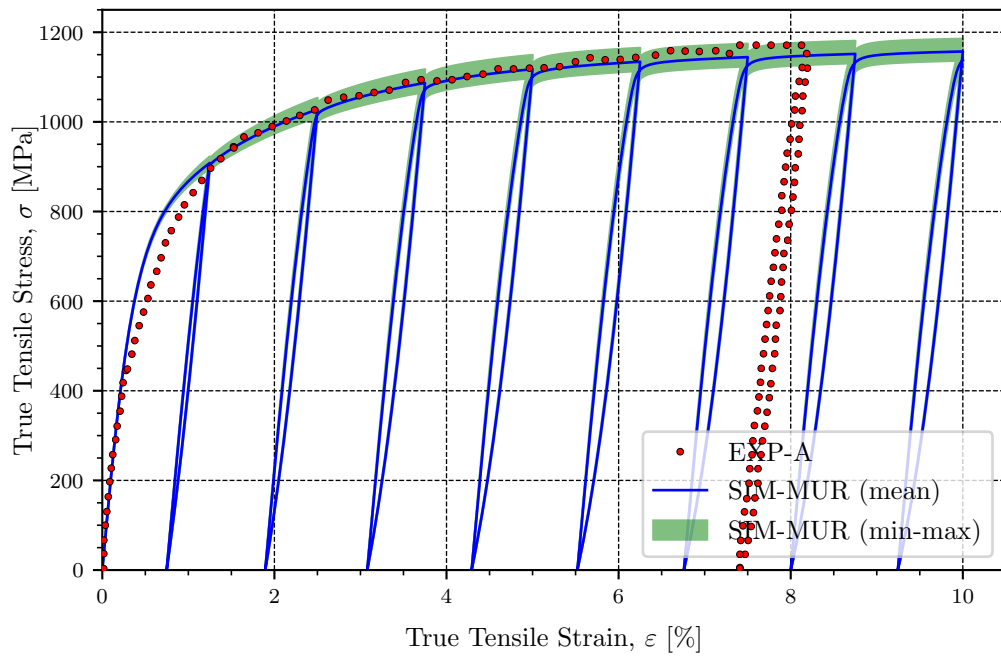


Figure 9: The simulation called SIM-MUR using the optimal input parameters (identified on data subset EXP-A). It includes several loading-unloading-reloading cycles that allow to evaluate the evolution of the moduli according to the prestrain. *The simulation labeled SIM-MUR uses the optimal input parameters (identified on sub-dataset EXP-A). The simulation SIM-MUR has multiple loading-unloading-reloading cycles to calculate moduli on each cycle and to evaluate the moduli evolution as a function of the prestrain.*

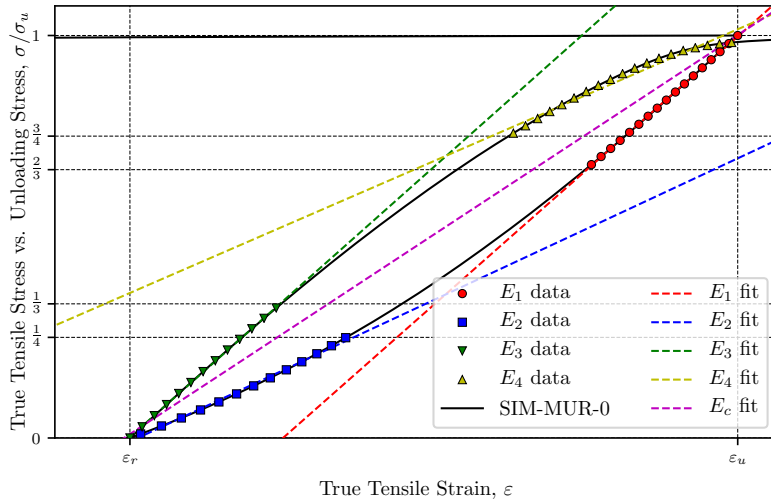


Figure 10: Schematical representation of the procedure introduced by *Chen et al.* (2016b) in order to calculate the 5 moduli E_1 , E_2 , E_3 , E_4 and E_c for each unloading reloading cycle. The vertical axis represents the normalized true stress σ/σ_u , where σ_u is the true stress at the beginning of the unloading step. Each modulus is defined as the slope of a linear fit obtained over a given subset of the data points depending on which modulus is calculated.

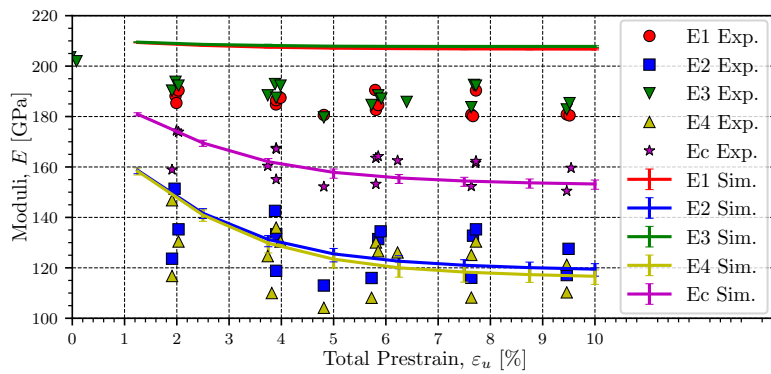


Figure 11: The evolution of the 5 apparent moduli calculated on SIM-MUR is compared to the experimental *Experimental data are* data extracted from Fig. 5 of *Chen et al.* (2016b).