



Learning the non-proportional multiaxial elastic–plastic response of an aluminium alloy with neural networks[☆]

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ABSTRACT

We present a surrogate model for the elastic–plastic response of an aluminium alloy, based on simple neural networks trained on measurements taken in tension–torsion and compression–torsion experiments. In these tests hollow cylindrical test specimens are subjected to pseudo-random time histories of applied axial force and torque. Multiple random experiments are conducted to explore the strain and stress space in both the elastic and elastic–plastic regimes of material behaviour. The corresponding histories of axial and shear stress and strain are subdivided in small increments, each of which representing a unit training datapoint. A surrogate model in strain control, based on feed-forward neural networks, is implemented; this comprises a classification network, which distinguishes elastic from elastic–plastic increments, and a regression network to compute the increment in stress as a function of the increment in total strain. The accuracy of the model is evaluated by predicting the material's response to random loading histories not included in the training dataset.

1. Introduction

In recent years, the integration of machine learning (ML) techniques in materials science and engineering has demonstrated great potential [1,2]. This trend is particularly evident in the field of computational [3] and experimental solid mechanics [4,5], where ML has begun to integrate and enhance traditional methodologies. In computational solid mechanics, ML has been applied in various studies, primarily aiming to reduce the computational cost of simulations by creating surrogate models [6,7] or data-driven microstructure-property relationships [8,9]. Notably, ML-driven models have been developed for path- [10,11] and history-dependent plasticity [12], thermo-viscoplasticity [13], hyperelasticity [14], and crystal plasticity [15]. Micromechanics approaches [16,17] and dislocation dynamics [18,19] have also benefited from machine learning applications. Some researchers have focused on the response of heterogeneous solids, specifically two-phase composites, using data-driven approaches to predict the effects of their microstructures on mechanical behaviour [20]. Additionally, more specific applications have emerged. For instance, Liu et al. [21] explored the mechanical response of graphene reinforced aluminium, utilizing molecular dynamics (MD), neural networks, and Halpin-Tsai models. Su

et al. [22] demonstrated the potential of machine learning to advance constitutive modelling of granular materials by developing a thermodynamics-informed neural network that integrates physical principles into a path-dependent recurrent neural network framework. These advancements illustrate the broad applicability of ML in enhancing the efficiency and accuracy of computational solid mechanics.

Experimental solid mechanics has also seen a growing interest in applying ML techniques to experimental data [23,24]. The learning capabilities of ML models, such as neural networks, allows direct utilisation of experimental data. Researchers have worked on data-driven models for elastic–plastic solids, collecting training data from measurements of simple loading histories [25]. More recent studies have explored various ML applications to model complex, history-dependant material behaviour [26], including temperature and strain rate dependency [27] utilising direct information obtained from experiments, obtaining models of high accuracy. For instance, Li et al. [28] developed a modified Johnson-Cook plasticity model to accurately capture the unconventional temperature and strain rate dependencies of dual-phase steel specimens. The model comprised a von Mises yield surface, an anisotropic flow rule, a reference stress–strain curve defining the rate-

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independent behaviour at room temperature, and a neural network function that depends on plastic strain, strain rate, and temperature. Sheng et al. [29] employed a ML approach to predict grain boundaries sensitive to damage nucleation, using in-situ tensile tests on samples with different textures. Cai et al. [30] investigated the concurrent effects of printing parameters and strain rate on the dynamic response of additively manufactured fibre reinforced bio-composites, and produced a data-driven model to predict the dynamic strength of the material as a function of the printing parameters and strain rate. Sangid [31] demonstrated the potential of integrating experiments and modelling to advance the understanding of plasticity and failure in polycrystalline metals by combining multi-scale techniques with in-situ experiments for improved model calibration and validation.

The existing research applying ML to experimental mechanics has examined simple loading conditions, often uniaxial loading or proportional and monotonic multiaxial loading. In this paper, we make a step towards the generalisation of a technique to extract constitutive models directly from measured data, for non-proportional multiaxial loading and in the absence of any underlying theoretical framework. We choose an aluminium alloy for this research, due to its wide range of applicability. The literature includes several valuable studies on aluminium constitutive modelling [32–34], including plasticity models focusing on non-monotonic loading under abrupt strain path changes [35]. In [36], we developed a strategy to obtain data-driven constitutive models from random experiments, demonstrating its feasibility via virtual experiments. In this study, we demonstrate a similar technique using real experimental data. We conduct novel mechanical tests, and we process the experimental data to form a training dataset for a machine learning exercise, with the objective of obtaining a data-driven surrogate constitutive model. We explore the case of multiaxial, non-proportional, non-monotonic loading on a widely used aluminium alloy.

The paper is structured as follows: Section 2 provides information about the design and execution of the experiments. Section 3 presents the implementation of the data-driven model. Results are presented and discussed in Section 4.

2. Design of the mechanical tests and data processing

2.1. Material and specimen geometry

Cylindrical bars of aluminium alloy 6082 grade T6, with 30 mm diameter, were obtained from Smiths Metal Centres, UK. Hollow, cylindrical, thin-walled specimens with axisymmetric geometry were manufactured using CNC subtractive manufacturing, following the design in Fig. 1. The inclusion of axisymmetric shoulders and hexagonal

ends served the purpose of facilitating the connection of the specimens to the loading fixture. The gauge portion was designed based on the finite element studies in [36–38], to ensure approximate uniformity of the axial and shear strains and to avoid compressive wrinkling and torsional buckling during the tests.

2.2. Experimental setup and procedure

The aluminium specimens were mounted to a steel loading fixture using hexagonal ends and circular shoulders on both extremities, as shown in Fig. 1. The fixtures were loaded by an electro-mechanical testing machine via mounting pins. The machine operated in load control; axial and torsional loadings were applied, and digital image correlation (DIC) was employed to measure the axial and shear strains within the gauge portion. DIC images, of resolution 2058 x 2456 pixel, were captured at a frequency of 1 Hz, while the loads were recorded at a frequency of 20 Hz. The full-field DIC measurements indicated a uniform strain field on the surface of the gauge portion. Three points within the gauge portion were tracked, and their measured position was used, after correction for the non-planarity of the surface and possible rigid body motion, to determine the histories of the axial, circumferential and hoop strain. The load was measured by resistive load cells of capacity 100 kN (axial) and 1000 Nm (torsional).

Twenty-six different specimens were subjected to random axial–torsional loading and one specimen was loaded in non-monotonic pure torsion. Each experiment consisted of 10 steps, in each of which tension–torsion or compression–torsion loads were imposed on the specimens. Each loading step was followed by an unloading step. The loading steps were designed to reach a sufficiently high target level of equivalent von Mises stress $(\sigma_{VM})_{2k-1}$, ($k = 1, 2, \dots, 5$), to ensure yielding; conversely, the unloading steps were designed to bring the equivalent von Mises stress below a target level, to ensure the material was left in the elastic regime at the end of each unloading step. For each step, a random combination of axial and shear stresses (σ_z and $\sigma_{\theta z}$, respectively) was calculated such to have

$$(\sigma_{VM})_{2k-1} = ((\sigma_{VM})_{2k-3} + 10)\text{MPa};$$

$$(\sigma_{VM})_{2k} = (r[-20, 0] + 200)\text{MPa};$$

$$(\Delta\sigma_z)_k = r[\Delta\sigma_{zmin}, (\sigma_{VM})_k];$$

$$(\Delta\sigma_{\theta z})_k = \sqrt{\frac{(\sigma_{VM})_k^2 - (\Delta\sigma_z)_k^2}{3}}. \quad (1)$$

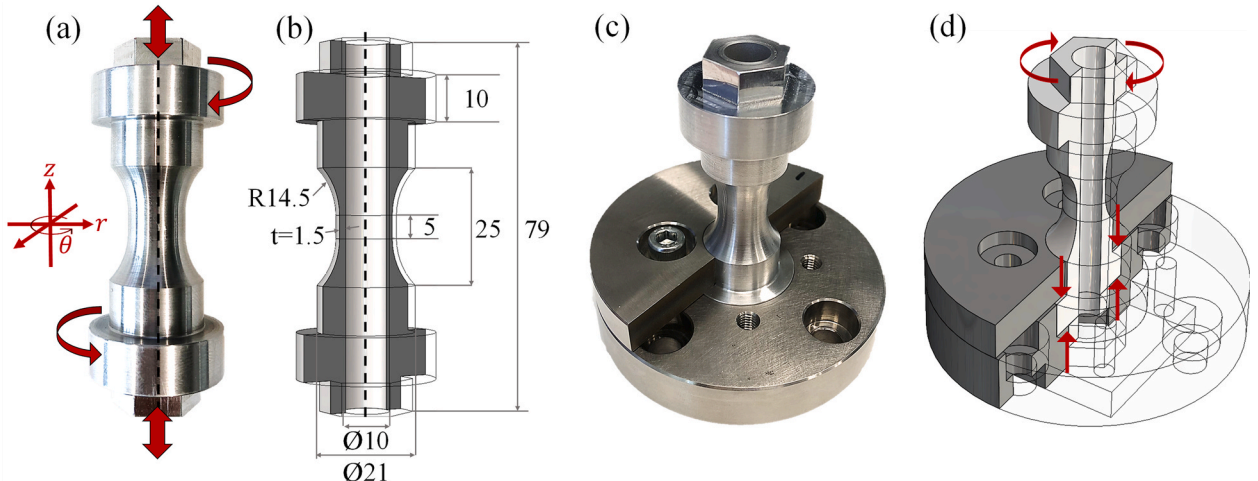


Fig. 1. Photographs (a)(c) and 3D rendering (b)(d) of the test specimens and their mounting in the loading fixture (all dimensions are in mm).

where $r[]$ is a uniform random number in the interval specified. The stresses quoted in eq. (1) were related to the applied loads by formulae for thin-walled circular cylindrical tubes, which were shown in [36] to be sufficiently accurate. The axial and torsional loads varied linearly with time during each of the 10 loading steps. Following a preliminary study, the first target value of the applied von Mises stress value was chosen as $(\sigma_{VM})_1 = 270\text{MPa}$, to ensure yielding. We also chose $\Delta\sigma_{zmin} = 20\text{MPa}$. The rates of axial and torsional loading were different but correlated, since the imposed axial and torsional loads were linearly ramped over time such as to reach their target values simultaneously (note: we will assume in the following that the material's plastic response was approximately rate insensitive in the quasi-static regime explored in this study). The loading history in eq. (1) were designed to ensure that the material's loading would lie outside the yield surface at the end of odd steps (loading) and within the yield surface at the end of even steps (unloading).

Fig. 2(a) illustrates the time histories of the applied von Mises stress imposed during the tests performed; Fig. 2(b) shows the details of the axial force and torque applied in a selected experiment, while Fig. 2(c) shows the path described in true strain space consequent to the application of the loads in Fig. 2(b). The conversion between nominal and true stresses and strains was conducted with the usual formulae for plastically incompressible solids, which involved calculating the principal stretch directions, taking the natural logarithms of such principal stretches, and reverting back to the original Cartesian reference system to obtain the true stress and strain tensors. The material exhibited the expected stress versus strain response, with elastic properties in the expected ranges. Preliminary checks, and the manufacturer's datasheet, indicated that the degree of transverse isotropy of the material was negligible for both the elastic and plastic responses. We therefore assume below that the solid was effectively isotropic.

A total of 27 non-monotonic experiments were carried out: 13 in tension-torsion, 13 in compression-torsion, and one in non-monotonic pure torsion. It would have been desirable to have experiments with axial loads spanning both the positive and negative axis, however this proved problematic due to slack in the mechanical coupling of the specimen and test machine, combined with the test protocol in load control. The choice of operating in load-control was driven by the availability of the test machine; a displacement-control test protocol would be preferable if the objective is to develop a strain-control constitutive model. The total of 27 specimens represented the maximum number of usable specimens that could be manufactured from a single metal bar, to eliminate the possible complications induced by the inevitable batch-to-batch variability.

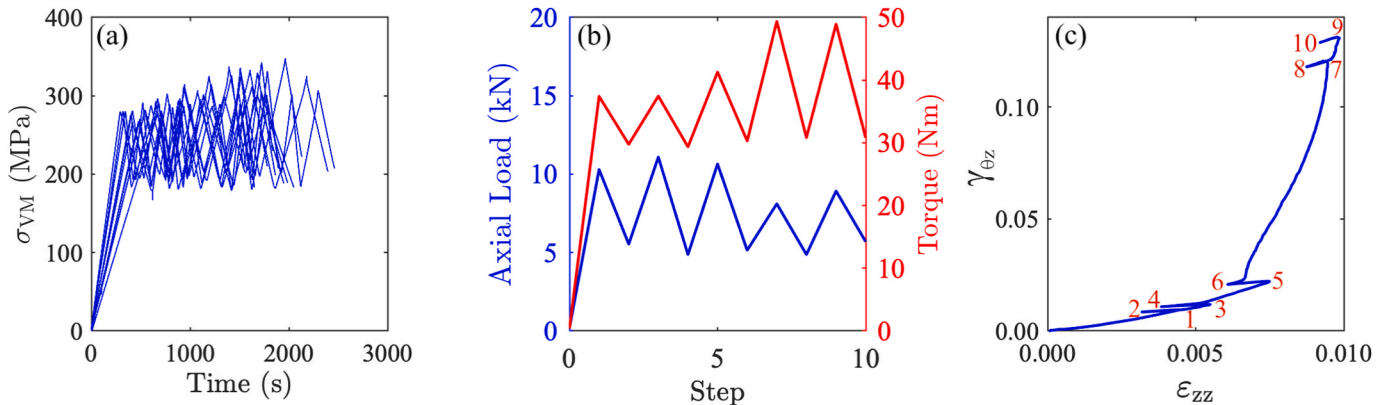


Fig. 2. (a) Time histories of the von Mises stress imposed in the experiments; (b) example of the force and torque histories imposed in a selected experiment; (c) projection of the path described in true strain space consequent to the loading history in (b).

2.3. Processing of the test data

An example of the recorded time histories of stress and strain for one selected compression-torsion experiment is shown in Fig. 3; some noise was present in the data, mostly due to the measurements of the (small) strains by image processing. Fig. 4 shows two examples of the raw experimental data for two experiments, chosen to illustrate the range of quality of the recorded data and the typical problems with these measurements.

In this figure one can observe problems with the measurement of axial strains at the beginning of the tests (specifically, an unexpected non-linear relation between stress and strain, due to slack in the mechanical coupling, introducing possible rigid body motion and affecting the quality of the images taken) as well as an apparent material softening, for example where marked by the red circles in Fig. 4. Such softening behaviour is likely due to creep of the material at high stress: the local peaks in the stress-strain curves correspond to the instant in time when the loading rate changed sign, i.e. to the transition between a loading step and an unloading step. While the magnitude of the load decreased as prescribed by the test machine, the magnitude of the strains initially kept increasing, to then start decreasing after a few seconds. As the surrogate model developed in this paper is intended to be rate insensitive and to operate in strain control, this apparent strain softening was undesirable. All of the undesirable features of the raw data were corrected before assembling the training database for the surrogate model. This involved the following steps.

1. The non-linear stress versus strain responses occasionally recorded at the beginning of some experiments were removed and replaced by linear stress-strain histories, and the strain axis was correspondingly shifted to ensure that all stress-strain histories had vanishing stress at the beginning of the tests (in the initial unstrained state).
2. Appropriate portions of the expected linear elastic regions (both at the beginning of the tests and during the unloading-reloading of the samples) were least-square fitted to straight lines, allowing the calculation of the Young's modulus and shear modulus. Such moduli showed a small variation across different tests and within each test ($<5\%$), with no apparent monotonic decrease with continued straining. This suggested that the material exhibited negligible damage; consequently, the surrogate model developed below will assume a material stiffness independent of strain. The actual stress-strain data in the elastic regions was replaced by perfectly linear relations according to the average of the measured Young's and shear moduli. The points where the measured stress-strain curves deviated from such linear behaviour were identified by human judgement and the corresponding stress and strain values were recorded.

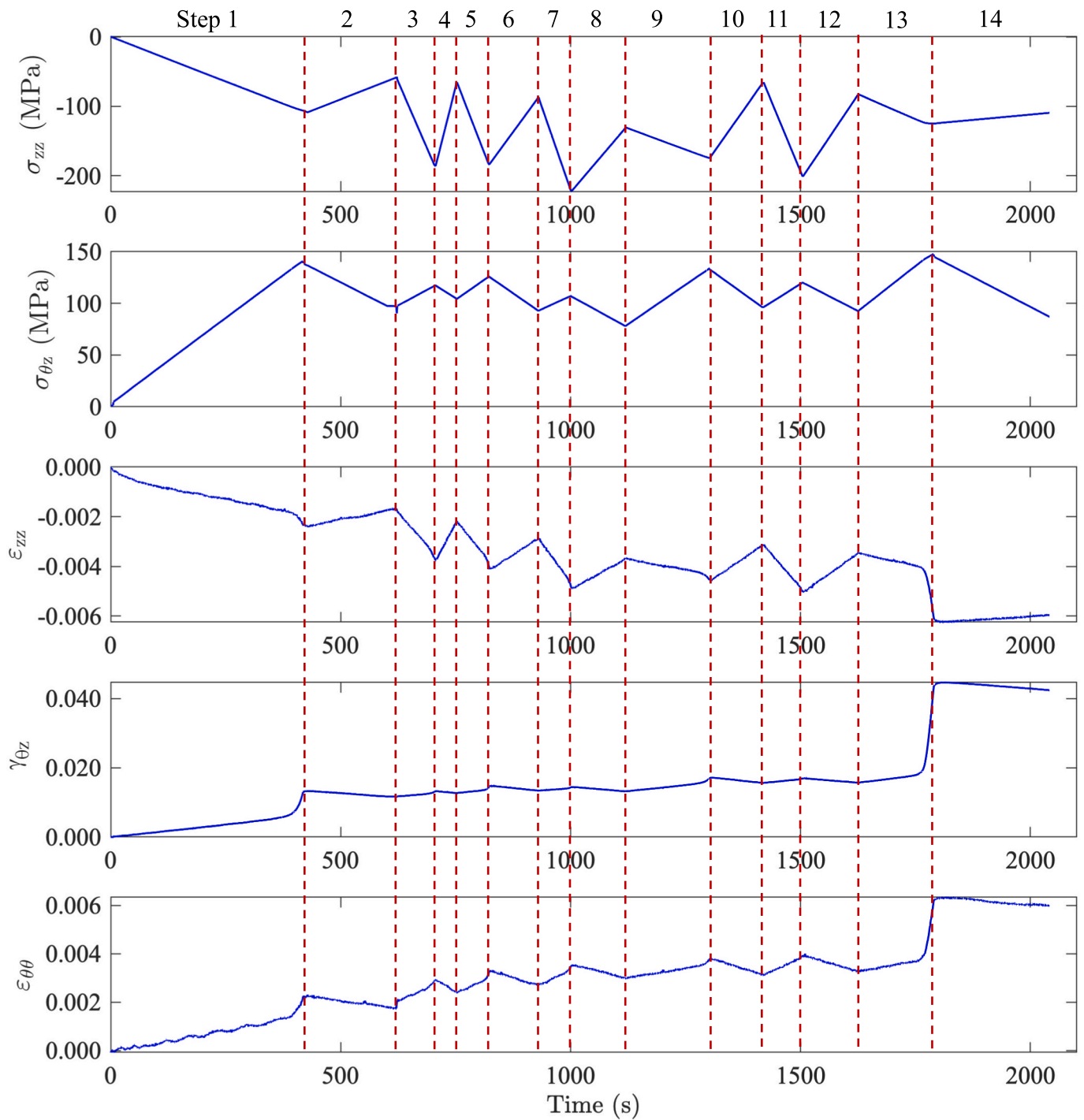


Fig. 3. Example of the measured stresses and strains histories in a selected experiment.

3. The regions of the stress–strain curves displaying apparent strain softening were removed and replaced by two straight lines: the first straight line had identical slope to the average slope of the actual stress–strain curve before the onset of softening; the second straight line had a slope equal to the average Young's or shear modulus, and merged with the subsequent elastic unloading data. This correction was selected among the many possible ones because of its simplicity.
4. The remaining nonlinear portions of the stress versus strain curves, corresponding to yielding and strain hardening of the material, were fitted with smoothing splines ensuring continuity of the slope of the stress–strain curves at the extremes of these nonlinear regions.

5. The measured histories of the circumferential strain versus time were split in subsets corresponding to the different loading steps, and each subset was fitted with a spline.

Fig. 5 presents, for a selected experiment, a comparison of the raw and processed data, to reassure the reader that the applied processing did not change the nature of the measurements, with the exception of the fact that the apparent strain softening was neglected; Fig. 5 however shows that the effect of creep on the test measurement is negligibly small. This problem could be completely eliminated by performing tests at constant strain rate in displacement control. The stress–strain curves were effectively split, during processing, into multiple subsets that were

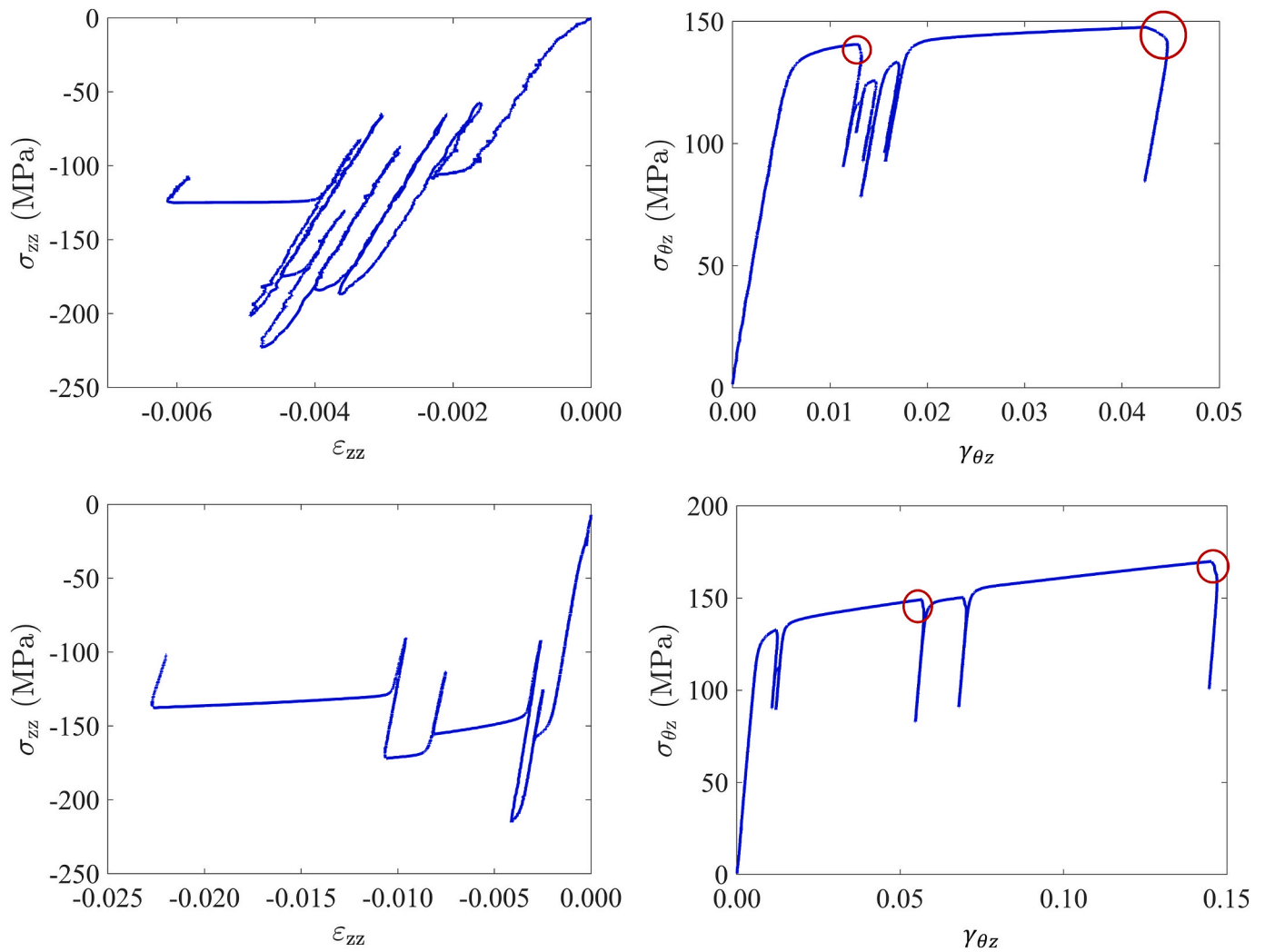


Fig. 4. Examples of the stress versus strain histories recorded during the tests. The upper row is for an experiment with relatively low magnitude of strains and therefore relatively less apparent noise in the axial strain measurement, compared to the lower row.

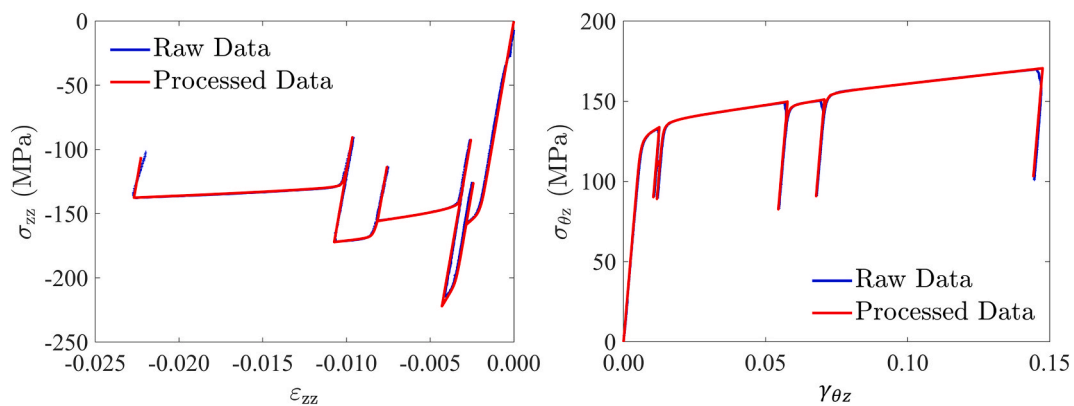


Fig. 5. A comparison of the raw and processed stress versus strain measurements.

known analytically. It was therefore easy to implement scripts to seed the curves with the desired time frequency, obtaining a set of ordered points of dimensionality 6 (time, two true stress components, three true strain components). The algorithm used preserved the physical time and could seed the curves with uniform or variable frequency, which is convenient for the application of machine learning to the data. In the results presented in the following however, a uniform time frequency

was used.

3. Surrogate model

3.1. Training data set

Fig. 6 visualises data from all 27 tests (excluding, for clarity, the

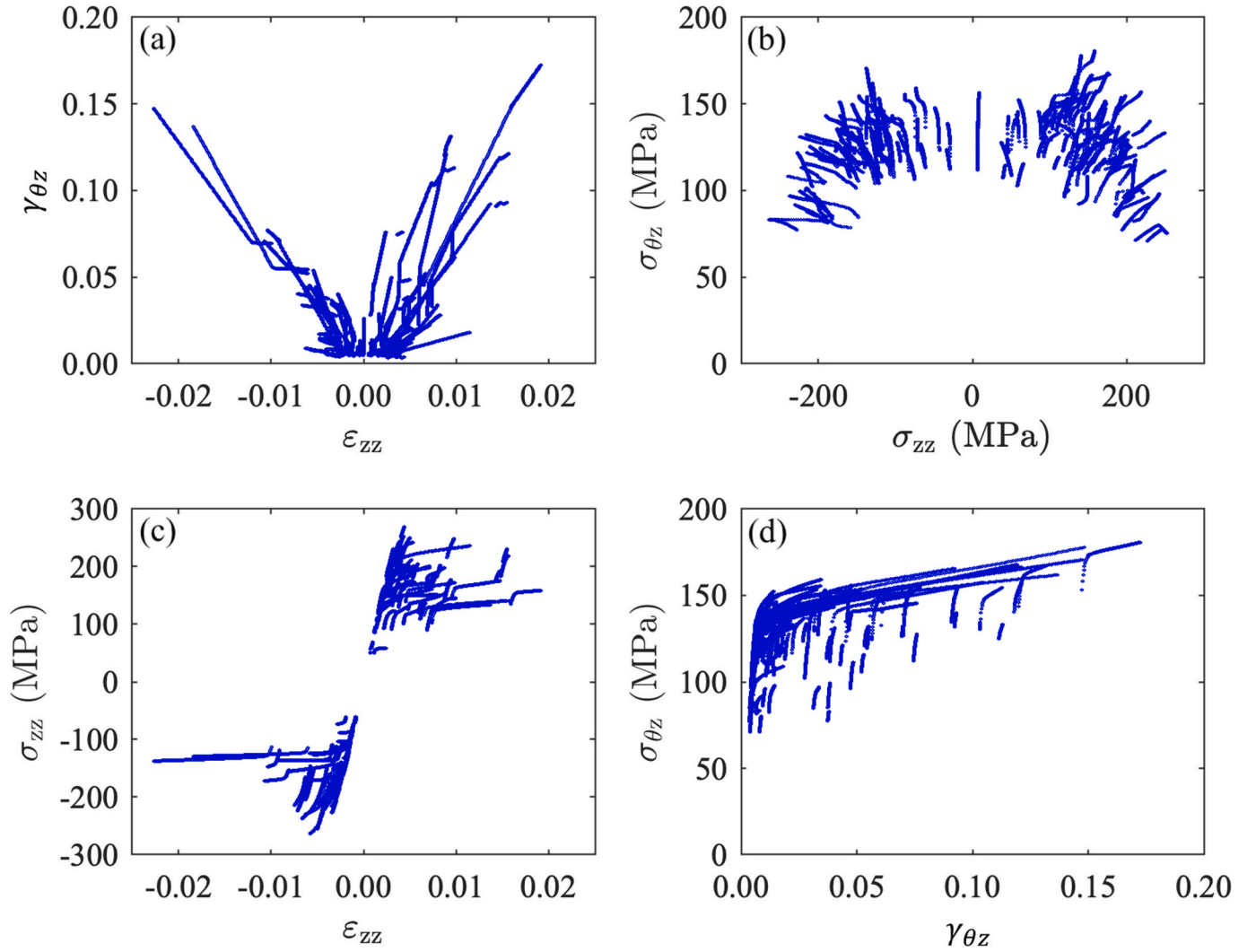


Fig. 6. Visualisation of the plastic increments composing the training dataset in strain space (a); stress space (b); axial stress versus axial strain space (c); shear stress versus shear strain space (d).

elastic portions of all the stress–strain curves measured) in strain, stress, and axial and shear stress/strain space. The data shown comprise approximately 11,000 datapoints. The distribution of the data in stress space is suggestive of an approximately quadratic yield function. In strain space, the data clearly appear denser at small strains, by the nature of the tests performed, which always started at zero stress and strain.

Pairs of consecutive datapoints were considered together to define an *increment*, and the surrogate model was designed to predict the evolution of different quantities across each increment. The current logarithmic strain vector, true stress vector, strain increment vector, and stress increment vector are defined as

$$\mathbf{e}_i = \begin{pmatrix} \epsilon_z \\ \epsilon_r = \epsilon_\theta \\ \epsilon_{\theta z} \end{pmatrix}; \mathbf{\sigma}_i = \begin{pmatrix} \sigma_z \\ \sigma_r = \sigma_\theta = 0 \\ \sigma_{\theta z} \end{pmatrix}; \Delta \mathbf{e}_i = \mathbf{e}_{i+1} - \mathbf{e}_i; \Delta \mathbf{\sigma}_i = \mathbf{\sigma}_{i+1} - \mathbf{\sigma}_i; \quad (2)$$

where i denotes the state at the beginning of the i -th increment and $i+1$ represents the state at the end of such increment. Considering the relatively small strains experienced by the specimens, we assume that additive strain decomposition applies, i.e.

$$\mathbf{\epsilon} = \mathbf{\epsilon}^{el} + \mathbf{\epsilon}^{pl} = \mathbf{S}\mathbf{\sigma} + \mathbf{\epsilon}^{pl} \quad (3)$$

where $\mathbf{S}$ denotes the compliance matrix, defined as

$$\mathbf{e}^{el} = \begin{bmatrix} S_{11} & S_{12} & 0 \\ S_{12} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{bmatrix} \mathbf{\sigma}. \quad (4)$$

The vanishing terms of the compliance matrix are justified by the absence of coupling between normal and shear actions in the material which is isotropic (or more precisely, slightly transversely isotropic); the lack of such coupling was confirmed in preliminary tests. Eq. (4) was used to convert the stress vector $\mathbf{\sigma}$ into the elastic strain vector $\mathbf{e}^{el}$, for all datapoints, and to calculate the increments in elastic strain $\Delta \mathbf{e}_i^{el} = \mathbf{e}_{i+1}^{el} - \mathbf{e}_i^{el}$ and in plastic strain, as $\Delta \mathbf{e}_i^{pl} = \Delta \mathbf{e}_i - \Delta \mathbf{e}_i^{el}$. We also calculated the equivalent von Mises stress σ_{VMi} and the accumulated value of the equivalent von Mises plastic strain $\bar{\epsilon}_i^{pl}$, as

$$\bar{\epsilon}_i^{pl} = \sum_{k=0}^i \Delta \bar{\epsilon}_k^{pl} = \sum_{k=1}^i \sqrt{\frac{2}{3} \Delta \epsilon_k^{pl} \Delta \epsilon_k^{pl}} \\ = \sum_{k=0}^i \sqrt{\frac{2}{3} \left[(\Delta \epsilon_{zz}^{pl})_k^2 + 8 (\Delta \epsilon_{\theta z}^{pl})_k^2 + 2 (\Delta \epsilon_{\theta\theta}^{pl})_k^2 \right]} \quad (5)$$

Each increment was assigned a Boolean flag value Y given by

$$Y = \begin{cases} 1 & \text{if } \Delta \bar{\epsilon}_i^{pl} \geq 2 \cdot 10^{-6} \\ 0 & \text{if } \Delta \bar{\epsilon}_i^{pl} < 2 \cdot 10^{-6} \end{cases} \quad (6)$$

with the intent of separating elastic from elastic-plastic deformation increments. $Y = 1$ corresponded to an elastic-plastic increment and $Y = 0$ corresponded to an elastic increment. The threshold of $2 \cdot 10^{-6}$ used in eq. (6) was determined by a numerical optimisation: it was found that using higher values for the threshold led to some clearly elastic-plastic increments being incorrectly categorised as elastic; on the other hand, using a lower threshold caused some clearly elastic increments to be mistakenly classified as elastic-plastic.

Fig. 7 shows the test data as histories of the equivalent von Mises stress versus accumulated plastic strain. This suggests a material that does not exactly follows J2 plasticity and displays some degree of kinematic hardening, as suggested in the literature [39]. An analysis of the increments where the variable Y first achieves a value of 1 during a specific test (i.e., of the onset of first yielding in different tests), together with the locus that such increments described in principal stress space, and the direction of the plastic strain increments, suggested that the material only approximately followed the normality rule. As expected, the material was also plastically incompressible as shown in Fig. 8, which displays the time histories, in all tests, of two of the individual normal plastic strain components together with the plastic volumetric strain.

Due to the scarcity of data, only 25 of the 27 tests performed were used to assemble the training dataset, while the remaining 2 (two randomly chosen tension-torsion and compression-torsion tests) were excluded from the training dataset and used for testing of the surrogate model. A preliminary investigation on the amount of training data revealed that data from at least 25 tests was needed to assemble a training dataset for a neural network of suitable accuracy. This left only two experiments to assess the accuracy of the surrogate model. Therefore, the model training was performed multiple times, each time excluding 2 experiments (one in tension-torsion and the other in compression-torsion) to be used to test the model's performance. All the increments from the 25 selected experiments were considered and split in two subsets in 80/20 % proportions, with 80 % of the data used in training and the remaining 20 % used in validation. The training dataset consisted of an ordered set of deformation increments recorded in the tests, with the associated changes in the values of total, elastic and plastic strains, stresses, accumulated equivalent von Mises plastic strain and von Mises stress.

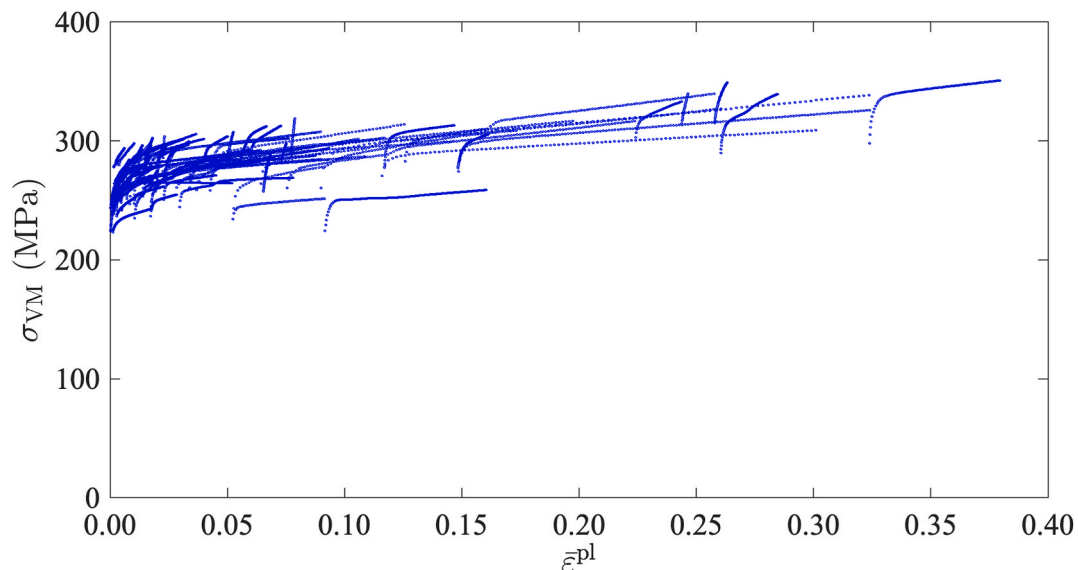


Fig. 7. Visualisation of elastic plastic increments in the von Mises stress versus accumulated von Mises plastic strain space.

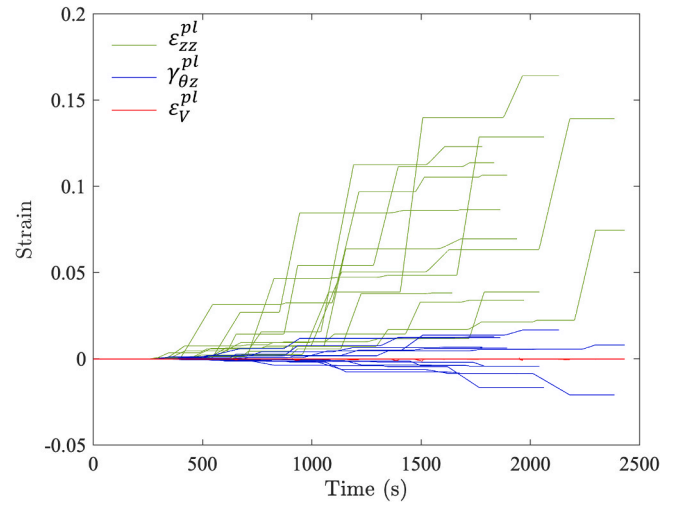


Fig. 8. Time histories of the plastic axial, shear and volumetric strains recorded in all experiments.

3.2. Surrogate model

The surrogate model was based on feed-forward neural networks (NNs) [40] implemented and trained in TensorFlow 2.15 [41]. Several model architectures were examined to capture the results of the measurements, including a surrogate model operating in load control and several different representations of the inputs and the outputs (such as using the principal invariants or the principal values of the elastic and plastic strain tensors). However, for brevity here we present only the most successful architecture, in which tensorial quantities were represented by their Cartesian components, and which operates in strain control, as required in potential applications in FE simulations. As shown schematically in Fig. 9, first a NN was used to separate increments into elastic or elastic-plastic categories, in a classification exercise; for elements classified as elastic, the model used the inverse of the compliance matrix to calculate the increment in stress from the increment in total strain (which coincided with the increment in elastic strain). For increments classified as elastic-plastic, a regression neural network was used to predict the increment in elastic strain, from which all strains and stresses, as well as the equivalent von Mises stress and accumulated plastic strain, could then be updated.

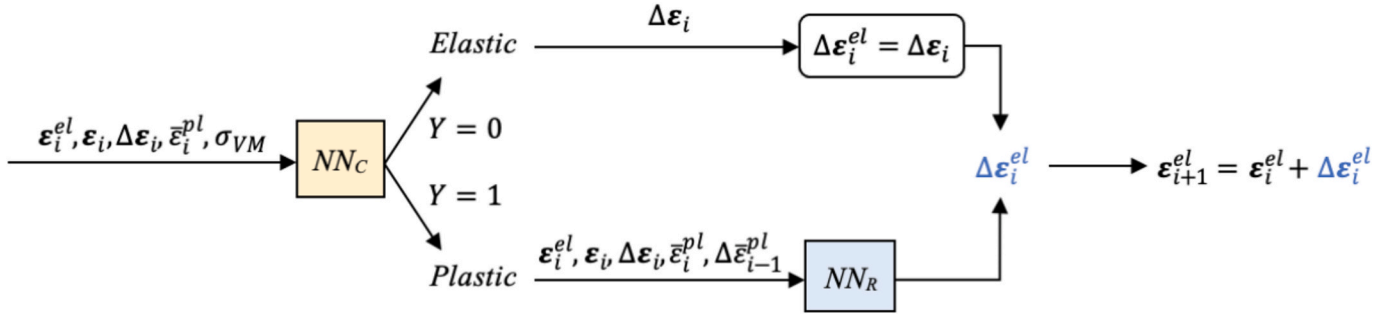


Fig. 9. Schematic of surrogate model.

The classification exercise shown in Fig. 9 is defined as

$$Y = NN_C(\epsilon_i^{el}, \epsilon_i, \Delta\epsilon_i, \bar{\epsilon}_i^{pl}, \sigma_{VMi}) \quad (7)$$

where Y is the flag defined in eq. (6), ϵ_i and ϵ_i^{el} represents the initial total strain and elastic strain, $\Delta\epsilon_i$ denotes the increments in total strain, $\bar{\epsilon}_i^{pl}$ is the accumulated plastic strain and σ_{VMi} is the equivalent von Mises stress. The model therefore uses as inputs the initial states of total strain and stress (represented by the elastic strain), the intended increment in strain, the initial accumulated Mises plastic strain, representing numerically the amount of statistically stored dislocations present in the material (quantifying the effects of loading history), and the initial Mises stress. We omitted considering the first principal invariant of the plastic strain tensor, as this was vanishing due to incompressibility (as shown in Fig. 8), and the third invariant of the strain tensor, as its inclusion was found in a preliminary study to reduce the overall accuracy. The model can deduce knowledge of the initial individual plastic strain components, which together with the accumulated Mises plastic strain and Mises stress provide (incomplete but) sufficient information to handle the shifting of the material's yield surface.

The hyperparameters of both classification and regression networks were determined by numerical optimisation. This involved exploring systematically the hyperparameter space in search of the highest overall accuracy of the surrogate calculations. A summary of all optimal hyperparameters is reported in Table 1.

The network NN_C comprised 2 hidden layers containing 32 neurons each. The inputs of NN_C were rescaled using the minmax() function; ReLU was the chosen activation function for the 2 hidden layers, while sigmoid [42] was used for the output layer; this architecture was selected by trial and error. A special dataset was assembled to train NN_C , by selecting an equal number of training datapoints (increments) with $Y = 1$ and $Y = 0$. The Binary Cross-Entropy (BCE) was the chosen loss function. The training of the NN was performed by backpropagation

using the Adam optimiser [43], a batch size of 100 and a learning rate of 0.001, and concluded within 3000 epochs. The analysis of the confusion matrix [44] showed that the classification had an accuracy of 100 % on the test data.

For elastic–plastic increments, the regression NN_R to predict the increment in the elastic strain increments was defined as

$$\Delta\epsilon_i^{el} = NN_R(\epsilon_i^{el}, \epsilon_i, \Delta\epsilon_i, \bar{\epsilon}_i^{pl}, \Delta\bar{\epsilon}_{i-1}^{pl}) \quad (8)$$

Similar to the case of NN_C above, ϵ_i , ϵ_i^{el} represent the current state of the material while $\bar{\epsilon}_i^{pl}$ is meant to quantify the effects of the previous history of plastic deformation, together with the initial elastic strain (equivalent to the initial stress). NN_R included among the inputs the variation of accumulated von Mises plastic strain in the preceding increment, $\Delta\bar{\epsilon}_{i-1}^{pl}$. Broadly speaking, this input helped the model realise if the material had just begun yielding or if the previous increments was already elastic–plastic. From the practical point of view, omitting it resulted in considerably worse predictions of the elastic strain increment at the transitions between elastic and elastic–plastic regimes.

The hyperparameters of NN_R were determined by trial and error. The final network had 3 hidden layers with 16 neurons each. All inputs and outputs were scaled by the minmax() function [44], and the hyperbolic tangent was the chosen activation function for all hidden layers (this was found to reduce overfitting compared to ReLU). The training of the NN was performed by backpropagation using the Adam optimiser [43], with a number of epochs set to 10,000, a batch size of 100 and a learning rate of 0.001. The Mean Absolute Error (MAE, [44]) was used as the basis of the loss function after a preliminary study. MAE is defined as

$$MAE(y) = \frac{1}{N} \sum_{i=1}^N |y_i - \bar{y}_i| \quad (9)$$

where N is the number of datapoints and $\bar{y}_i$ are the outputs predicted by the NN. The loss function was defined pragmatically by trial and error to maximise the accuracy, and the final loss was chosen as

$$5 MAE(\Delta\epsilon_{zz}^{el}) + MAE(\Delta\epsilon_{\theta\theta}^{el}) + MAE(\sigma_{VM}) \quad (10)$$

The weight factors of 5:1:1 for the three terms in eq. (10) were decided following a numerical optimisation. Both the higher weight placed on the axial strain increment and the inclusion of the von Mises stress term was found to substantially improve the network's ability to predict the stress/strain behaviour, in particular immediately after yielding.

3.3. Testing of the predictive ability of the surrogate model

To evaluate the accuracy of the model's predictions, we proceeded as follows. In turn, two experiments (one compression-torsion and one tension-torsion, randomly selected) were excluded from the training data and set aside to test the model's generalisation capability. This was repeated 3 times, to test the model's predictions on a total of 6 unseen multiaxial experiments (here 'unseen' is intended as an experiment not

Table 1
Summary of the optimal choice of hyperparameters in this study.

	NN_C : Classification		NN_R : Regression	
	Number of nodes	Activation function	Number of nodes	Activation function
Input layer	8	—	8	—
Hidden layer 1	32	ReLU	16	Tanh
Hidden layer 2	32	ReLU	16	Tanh
Hidden layer 3	—	—	16	Tanh
Output layer	1	Sigmoid	2	—
Loss function	Binary Cross-Entropy (BCE)		Mean Absolute Error (MAE)	
Optimiser	Adam		Adam	
Batch size	100		100	
Epochs	3000		10,000	

included in the training dataset, i.e. a test of which the surrogate model has no awareness).

The axial and shear strain histories of the unseen experiments were discretised in a set of ordered strain increments $\Delta\epsilon_i$, using a uniform time increment Δt equal to that used to produce the training dataset. All quantities were initialised as 0, and the surrogate model was used to predict the evolution of all quantities over the first increment $\Delta\epsilon_0$. All quantities were updated and the process repeated iteratively, with the surrogate model predicting the evolution of stresses as a function of strain.

The numerical value of the loss function used quantifies the model's accuracy in predicting the evolution of relevant quantities over a single increment. We note however that the loss function is not representative of how the model will perform in predicting the stress consequent to a

complex history of non-proportional and non-monotonic imposed strain; this is because any error made by the surrogate model over a particular increment will be carried on in the predictions of following increments; in addition, the stress versus strain predictions also depend on the performance of the classification model. Therefore, the accuracy of the model was quantified by considering the axial and shear stress versus strain curves, and for each extracting the Mean Absolute Percentage Error (MAPE), defined as

$$\text{MAPE}(y) = \frac{1}{N} \sum_{i=1}^N \left| \frac{y_i - \bar{y}_i}{y_i} \right| \quad (11)$$

The optimal choice of architecture and hyperparameters corresponded to the predictions with the highest value of MAPE, which will be presented below.

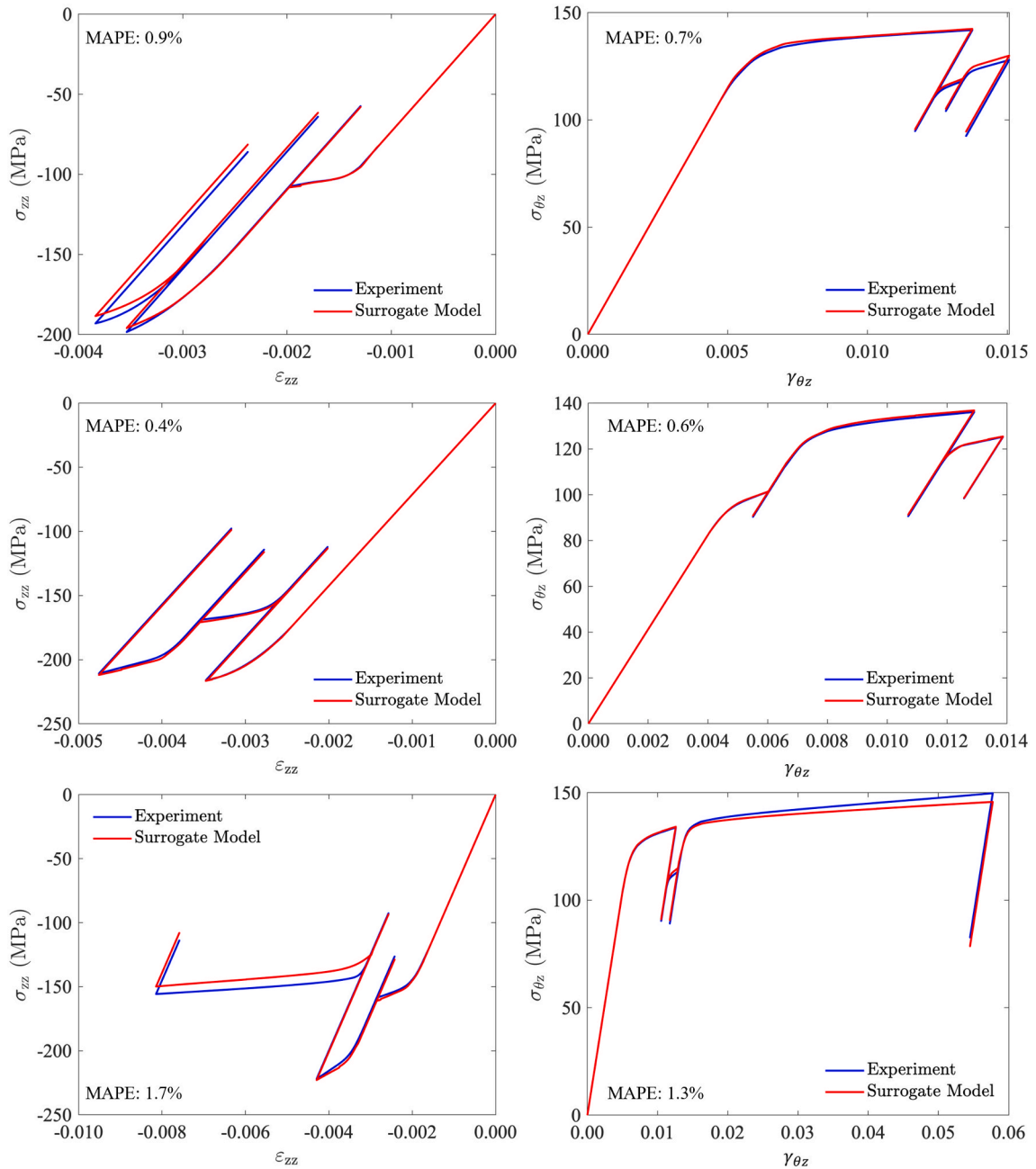


Fig. 10. Stress-strain histories corresponding to the three compression-torsion validation experiments used to assess the surrogate models; the left column shows measurements and predictions of the axial stress versus axial strain histories; the right column shows measurements and predictions of the shear stress versus axial strain histories. Each row refers to a different experiment.

4. Results and discussion

Fig. 10 and Fig. 11 display the stress–strain curves predicted by the surrogate model for the sets of three unseen (not included in the training database) random compression–torsion experiments and three unseen tension–torsion experiments, respectively. The predictions are compared with the measurements over the first 6 loading steps out of the 10 available, and the MAPE is calculated over the portion of the stress–strain curves shown in the figures. The model was found to be in very good agreement with the experimental data, achieving an average MAPE of 0.93 % for the three tension–torsion tests and of 0.66 % for the three compression–torsion tests. The model has similar accuracies in predicting the axial and shear stress versus strain curves; the comparison between measurements and predictions indicates that the classification

NN performs relatively better than the regression NN, as the transition between elastic to elastic–plastic regimes is always predicted correctly, while some discrepancies are seen, at the later stages of deformation, between the measured and predicted strain–hardening. As expected, the errors tend to increase with continued deformation; this is due to two factors: i) that errors made in a certain increment will be carried on in the subsequent increment, and ii) that as shown in Fig. 6, the density and uniformity of the data is lower for larger applied strains.

The data shows that the accuracy is progressively lost as the model starts operating in regions of the input space with lower and lower data density. Nevertheless the error is quite low in consideration of the complexity of the imposed strain histories. Such strains histories only comprise 6 steps, of which 3 are elastic–plastic and 3 are of elastic unloading; yet the human mind struggles to interpret and justify the

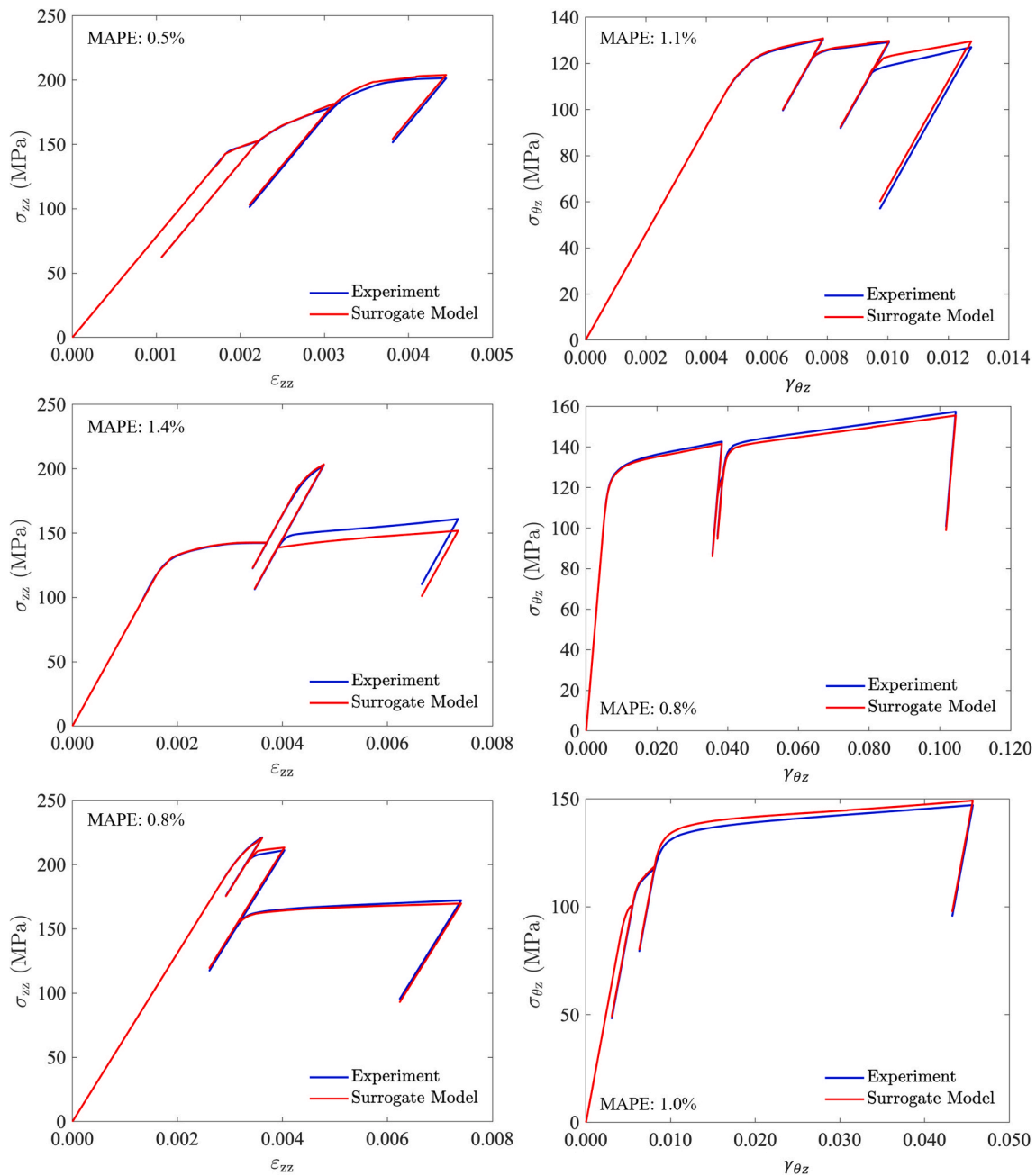


Fig. 11. Stress–strain histories corresponding to the three tension–torsion validation experiments used to assess the surrogate models; the left column shows measurements and predictions of the axial stress versus axial strain histories; the right column shows measurements and predictions of the shear stress versus axial strain histories. Each row refers to a different experiment.

material's response, a job that the data-driven model performs very comfortably.

The scarcity of data in our application resulted in the fact that we did not perform (and therefore did not include in the training) classical tests like uniaxial compression and tension. The surrogate model predicts a first yield at a stress of 242 MPa and 250 MPa in uniaxial tension and compression, respectively. This is in line with the data in Fig. 7, which shows an initial yield at a von Mises stress between 230 and 250 MPa for all experiments at multiple triaxialities, and in general in agreement with the published data for this material. For engineering applications of this aluminium alloy, most practitioners would opt to conduct monotonic tension tests, more rarely accompanied by monotonic torsion tests, and these monotonic uniaxial test results would lead to the conclusion that the material follows the von Mises criterion; typically J2 plasticity with isotropic hardening would then be selected as a constitutive model, for its ready availability in FE solvers and ease of calibration. Such modelling approach would lead to errors much higher than those made by the data-driven model in Fig. 10 and Fig. 11: for example it is clear from the graphs that the material does not yield at a given von Mises stress, nor at a von Mises stress monotonically increasing with the accumulated plastic strain, as also shown in Fig. 7. We argue here that the common practice of characterising a material's response performing proportional and monotonic mechanical tests may not be an efficient use of material and resources; while these tests are easy to interpret and may be insightful when developing theoretical models, very little information is harvested from the test data, when compared to the pseudo-random non-proportional and non-monotonic experiments proposed here, which explore, in a single mechanical test, much more of the input space defining the material's response.

We also observe that the data-driven model makes no theoretical assumption on the material's response, with the exception of rate-independence, which could be relaxed by exploring the sensitivity to strain rate in the tests (as shown for example in [45], an exercise that was not deemed necessary for this particular solid). We further assume that tests are isothermal, as it can be easily checked experimentally [46]. The transverse isotropy of the solid and the absence of damage was observed directly from the data, however, in cases where these two assumptions should not hold, similar data-driven surrogate models could also be derived for ductile solids displaying damage [47] and with arbitrary anisotropy [48], subject to the existence of damage-related data obtained by employing appropriate experimental techniques [49]. Our choice of inputs and outputs is only driven by the data, namely by the fact that the solid is plastically incompressible and the stress state is two-dimensional. The inputs chosen are insufficient to completely define a plastic response displaying a combination of volumetric and kinematic hardening, nevertheless the model is effective in capturing the effects of both the shifting and growth of the yield surface.

The model presented is not "physics informed": not only no assumptions are made on the type of flow rule and shape of the yield surface, but we do not even enforce the first two laws of thermodynamics or use arguments of material symmetry or convexity. Nevertheless, the data does always satisfy these physical principles and our simple NNs learn them with ease by induction bias. In contrast, when developing theoretical phenomenological or micromechanical models, a vast number of assumptions needs to be made, mainly in pursuit of simpler mathematical treatments and experimental calibration, resulting in less flexibility (and therefore accuracy) of the final model.

The data-driven model presented here has the same form as the incremental constitutive models used in FE simulations, and it can be readily incorporated in a material subroutine for any commercial or bespoke software, as we demonstrated in [36] by writing a UMAT subroutine for Abaqus based on a NN. In particular when used with implicit FE solvers, a data-driven model has the further advantage that it performs direct predictions of the stress increments as a function of the strain increments and other state variables, without the need for iterative procedures, which are required by conventional theoretical/

phenomenological models. We showed in [36] for example that a NN constitutive model can outperform the constitutive model for J2 plasticity built-in in Abaqus in computational speed, as the lack of iterative procedures remedies the higher number of operations required to evaluate the outputs of a NN, when compared to the simple equations of von Mises plasticity. The model presented in this study can be used to predict effectively the non-linear response of a 3D beam subject to arbitrary combinations of axial, bending and shear loadings, but it is limited to this scenario as it carries the limitations of the dataset used for training. We finally note that data-driven models based on directly measured data, which are shown here to be effective for a specific, widespread engineering metallic alloy, can offer even greater advantages in the case of novel materials of recent development, for which a deep understanding of the deformation mechanisms, and the corresponding theoretical or numerical predictive models, may be lacking.

4.1. Limitations of the study and future work

The experiments and modelling presented in this paper cannot result in a general constitutive model able to predict the material's response to a six-dimensional strain increment; the model in this study can, however, form a very fundamental part of such general AI model, which should be pursued by producing additional data in different regimes of the material's response, and by combining the model presented here with additional data-driven, phenomenological or micromechanical models (not excluding numerical simulations explicitly modelling the material's microstructure), for example using knowledge-based machine learning and ensemble learning; we shall demonstrate this in our future studies.

The total number of 27 experiments available in this study to form the training dataset was limited by external constraints. Our previous experience in [36], using data from virtual experiments, suggested that 50 tests was an adequate number to obtain sufficient accuracy. In the training experiments the strain rates experienced mild variations, however these were not embedded in the structure of the model, which was assumed to be rate-insensitive; this is consistent with the literature, which reports a very low strain rate sensitivity for the response of the 6082-T6 Al alloy [50]. Consequently the model's predictions can only be accurate at the low strain rates experienced in the training experiments. To extend the model's predictive ability to larger strains, the possibility of damage should be considered, which would imply a different architecture of the surrogate and would necessitate of quantitative data on the current material stiffness; this remains a challenge to address in future research.

5. Conclusions

We presented a novel experimental technique to obtain quantitative data on the elastic-plastic response of solids to non-proportional and non-monotonic multiaxial straining, based on tension/compression-torsion experiments on axisymmetric dogbone specimens with gauge portions in the form of thin-walled circular cylinders. The technique involved the application of pseudo-random non-proportional and non-monotonic loading to the specimens and the recording of the time histories of all the non-zero components of stress and strain. The recorded data served as a training dataset for a novel data-driven surrogate model to predict the increment in stress components as a function of an imposed increment in strain components. The model was based on simple feed-forward NNs and included a classification NN, to distinguish elastic from elastic-plastic increments, and a regression NN to predict the material's strain hardening in elastic-plastic increments. The model assumed a rate independent material response and absence of damage (justified by the small strains and strain rates applied, and by the existing literature on the 6082-T6 aluminium alloy investigated) but no further theoretical assumptions on the material behaviour were made. The data-driven model was found to be very effective in predicting the

axial and shear stress versus strain histories of the material subject to the application of pseudo-random axial and torsional loadings, achieving average errors typically less than 1 % over complex multiaxial experiments.

CRedit authorship contribution statement

Burcu Tasdemir: Writing – original draft, Software, Investigation, Formal analysis, Supervision. **Antonio Pellegrino:** Writing – review & editing, Supervision, Methodology, Funding acquisition. **Xinyu Su:** Investigation, Software. **Vito L. Tagarielli:** Writing – review & editing, Supervision, Methodology, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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