Low cycle fatigue life estimation by crystal plasticity and machine learning

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Abstract

An essential part of estimating low cycle fatigue life of an engineering component undergoing complex cyclic loading is establishing an accurate response of the material to cyclic loads with constant strain. Often, the resulting hysteresis loop is defined via semi-theoretical equations such as those proposed by Armstrong-Frederick (Frederick and Armstrong 2007) or Lemaitre-Chaboche (Lemaitre and Chaboche 1990). However, such models are either too simplistic and cannot accurately predict the cyclic response of the material or so complex that require large experimental programmes to calibrate them to the point, the experimental results are sufficient for prediction of material response.
An alternative approach is devising a numerical model that represents the right micromechanical physics of cyclic behaviour so it can accurately predict the response of the material and use it to predict the micromechanical hysteresis at different strain ranges. The first step in this approach is to identify the micromechanical physical parameters that influence the macromechanical response. While there are many parameters that play a role in cyclic behaviour, the key variables for macromechanical hysteresis loop are the evolution of kinematic and isotropic hardenings which implicitly capture the evolution of the Bauschinger effect. Crystal plasticity finite element simulations are well suited to capture these two parameters as the constitutive law includes formulation for hardening thus accounting for the isotropic behaviour. The hardening can be defined in a phenomenological fashion(Ashraf et al. 2024) or a more physics-based approach such as strain gradient plasticity (Dorward et al. 2024) can be used. These models represent the hardening of the material and often are suitable for monotonic deformations even to high levels of plasticity such as forming.

However, the kinematic hardening as observed in the case of cyclic loading is less studied and harder to represent. It could be argued that the key mechanism for hardening is intergranular (back-stress) and intragranular stresses also referred to as type III and type II residual stressed (Withers 2007). Crystal plasticity finite element frameworks inherently capture the intragranular residual stresses as the difference in the compliance of grains due to their orientation with respect to loading direction is accounted for thus, upon unloading the misfit between grains automatically simulates type II residual stresses. Type III residual stresses on the other hand must be explicitly formulated. While micromechanical rules such as the gradient of the distribution of geometrically necessary dislocations have been proposed (Bayley, Brekelmans, and Geers 2006) for modelling type III residual stresses, their measurement is not straightforward due to large uncertainty in distribution of geometrically necessary dislocation whose derivative becomes unreliable.

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Since the final aim of our model is to extract macromechanical properties, we have used a set of phenomenological constitutive laws with less influential micromechanical parameters captured via physics-based calibrating parameters. For example, the kinematic hardening has been modelled via one parameter that captures back stress in the material and can be calibrated via synchrotron X-ray diffraction. Inevitably by reducing the microstructural reliance of the model, its predictivity becomes limited. However, it reduces the complexity and therefore reduces the computational cost.

Despite the computational savings made in the model by moving towards a phenomenological constitutive law with combined calibrating parameters, it is still too complex and time-consuming to produce and solve model of a size which is comparable to that of an industrially relevant component. It therefore has a similar problem to a fully experimental approach, to run the model enough times to cover the full solution envelop, it will be computationally unfeasible although at much lower cost compared to experimental programmes.

The next step therefore is to reduce the computational cost of such complex models. We have employed a machine learning algorithm, that is Gaussian Process, to do this. Gaussian process regression predicts a conditional probability at each testing datapoint therefore giving an estimate for the output value and a variance at each point. The relationship between points in the input variable space can be described by a kernel function which for our case, we used a second order polynomial. Since the response of the material to cyclic loading is complex, first we used Functional principal component analysis (fPCA) to deconstructs the materials response (i.e. each half hysteresis loop) into a set of basic functions parameterised by scalar constants thus reducing the model that predicts the response. We could estimate the cyclic behaviour at each cycle by a combination of only 4 basic functions thus the Gaussian Process needed to predict 4 scalers for each half cycle for each strain condition.

After producing the surrogate model of the crystal plasticity framework, the model was tested against a set of experimental programme carried out previously on stainless steel 316H at 550oC. The experiments were uniaxial low cycle fatigue experiments with either constant strain ranges (between -0.6% to +0.6%) or variable strange ranges. The model performed well in predicating this behaviour. To make the model accessible by engineers, UHARD within ABAQUS. While the Abaqus simulations with UHARD could implement the model for industrial applications, it is currently limited to uniaxial conditions only not able to predict the evolution of yield surface in the case of multi-axial loading correctly. We therefore plan to expand the surrogate model to multi-axial condition, requiring defining a full 3D scale UMAT for all possible combinations of cyclic loadings in three dimensions.

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