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PREDICTING THE MACROSCOPIC CYCLIC BEHAVIOUR OF POLYCRYSTALLINE STEELS BASED ON MATERIAL MICROSTRUCTURE VIA SURROGATE MODELLING

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Abstract
Crystal plasticity finite element models can simulate the effect of microstructure on the cyclic behaviour of polycrystalline steels and can simulate the resulting local plastic strain. However, such models are computationally expensive and are therefore limited to simulation on small volume elements of material. In this work, a Gaussian process regression model is proposed as a surrogate model to predict macroscopic quantities of interest based on input parameters relating to the cyclic loading and material microstructure. The advantage with relation to computational expense of the surrogate can be leveraged for the purposes of undertaking uncertainty quantification and sensitivity analysis regarding the effect of the model inputs on the output prediction.

1. Introduction
Significant progress has been made in developing detailed mesoscale simulations of material behaviour that account for the effect of microstructural parameters on phenomena including cracking, fatigue and corrosion. Such simulations are of value in structural integrity relating to polycrystalline stainless steel alloys particularly in nuclear reactor plant coolant piping. Crystal plasticity models can be implemented within finite element solvers to model the behaviour of representative volume elements (RVEs) of material. Many crystal plasticity models include backstress evolution equations which account for kinematic hardening and the Bauschinger effect in polycrystalline materials under cyclic loading. Capturing these effects is crucial to understanding the evolution of local stress and plastic strain fields which in turn have an effect on the fatigue crack behaviour.

Crystal plasticity finite element (CPFE) models, however, are very computationally expensive and as a result are only capable of simulating small volume elements of polycrystalline materials. Typically these volume elements are on the order of microns. There has been an increasing interest recently in developing surrogate models, sometimes known as response surface models, which can emulate the response of computationally expensive complex simulations. Such surrogate models can be evaluated much more quickly than the complex models they aim to emulate. The relative speed of these models also yields advantages for uncertainty quantification, sensitivity analysis and CPFE model calibration where many complex model evaluations are typically required.

In this study, a Gaussian process (GPR) regression model is used to emulate the response of a strain gradient CPFE model under cyclic loading. Macroscopic quantities of interest such as the homogenised yield stress of the ensemble are extracted for models with different cyclic strain ranges, numbers of cycles and microstructural parameters.

2. Results
Monotonic tensile curves have been extracted from a strain gradient CPFE model for two instances of changing input parameters:

a. Changing the crystal plasticity parameters inputted to the CPFE
b. Changing the average diameter of grains in the RVE

For each instance, the yield stress is calculated for each simulation from the tensile data to form the output of the dataset.

In both instances a GPR model is created to approximate the yield stress given by the CPFE model for new unseen input data points. Figure 1 shows a visualisation of the GPR model predicting the yield stress of a

RVE based on the average grain diameter. The training data in this instance is stochastic in nature due to the random generation of the RVE at each input data point. The mean prediction from the GPR model as well as the 95% credible interval showing the epistemic uncertainty in the GPR prediction.

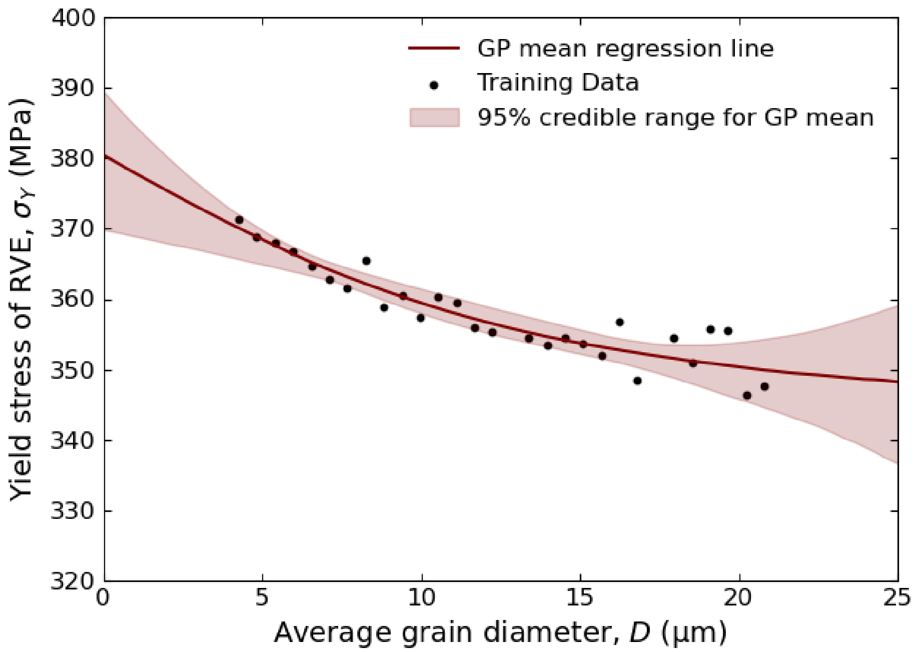

Fig.1 – Visualisation of the GPR model generated to predict yield stress based on the average grain size of an RVE of polycrystalline material.

The same strain gradient CPFE model has also been used to successfully model the cyclic behaviour various RVEs under different strain ranges and number of cycles. The same GPR methodology is to be applied to the cyclic model in order to provide a tool for quick estimation of outputs based on different strain rates, strain ranges, number of cycles and microstructural parameters.

3. Discussion

- Leave-one-out cross-validation is used to validate the predictive capability of the GPR model shown in Figure 1 resulting in r-squared scores >0.9.
- The GPR methodology has been shown to be able to deal with a higher number of input variables in other studies.
- Using a GPR model as a surrogate model allows for efficient model evaluation providing opportunities for sensitivity analysis, uncertainty quantification and calibration which typically require a large number of model evaluations.
- The ability of such methods to predict macroscopic behaviour of materials under both monotonic and cyclic loading based on different microstructural parameters is advantageous in beginning to bridge different material lengthscales.

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