In-silico Qualification of Materials

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Abstract

Material qualification is an important pre-requisite for design substantiation of any power plant. Historically, this is achieved through large experimental programmes that are eventually collated to support design standards (e.g. ASME) or later in assessment codes (e.g. UK's R5 and R6). This process is slow and expensive but low risk. In parallel, computer simulations have expanded their roles in the design and assessment process. Advanced physics-based simulations techniques such as crystal plasticity frameworks are increasingly being used to inform the engineering practices. However, they require extensive research to validate and substantial training for the practitioner to ensure the validity of their results. They are therefore considered to be expensive techniques that are deployed at exceptional circumstances. In this paper, a road map to use recent advances in machine learning is proposed that can simplify the complex physics-based simulations and produce high fidelity surrogate models that can be used cheaper, faster, with less stringent training. The surrogate models, because are based on rigorous physics-based simulations, can form part of the material qualification thus accelerating the process and making it more efficient.

1. Method

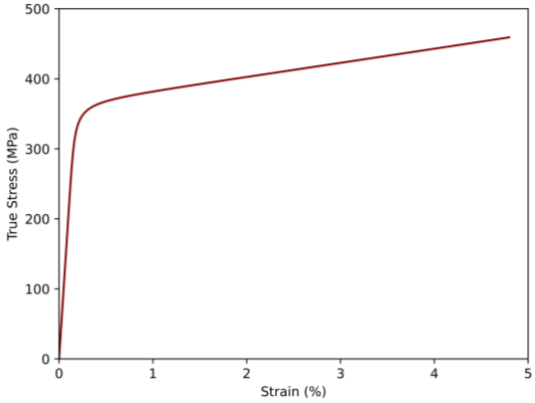
A strain gradient crystal plasticity framework was used in which the length scale (e.g. grain size) was intrinsically accounted for through the strain gradient forming at grain boundaries thus simulating pile-up that has been suggested in some cases to be an explanation for the Hall-Petch phenomenological observation between grain size and yield stress. The gradient plasticity crystal plasticity framework was implemented in ABAQUS and calibrated for stainless steel 316L(N) in its as-manufactured conditions. An experimental programme including tensile and room temperature cyclic were carried out results of which were used in calibrating the simulation constitutive law. A large number of model parameters which were dependent on micromechanical measurements (e.g. initial statistically stored dislocations, effective radius of backstress, mean-free path hardening factor, and annihilation rate) were extracted from literature and fixed. Only the critical resolved shear stress and the evolution of back stress as a function of yield point loci were calibrated. These are important values for prediction of creep-fatigue life of a high temperature component using assessment codes such as R5. This assessment has been shown to be one of the most life limiting factors in the UK high temperature gas-cooled plants.

The physics-based model is complex and time-consuming. While it can be used to inform assessments, it cannot be used to estimate the life a component with complex geometric features and loading multi-axiality and gradient as it only efficient to run on a representative volume element. In order to show the efficiency of machine learning algorithms to produce a reduced model of physics-based simulation, an example was used. In this example the input to the model was the size of the material grain and the output was the yield stress. The Sobol sequence was used to create a sample of average grain diameters between 3-20μm. These values are selected to keep the minimum number of grains greater than 100 in a 40x40x40 element RVE. The software DREAM.3D was used to construct random microstructures with the given average grain diameters. Boundary conditions are imposed on the CPFE model to simulate simple tension. The data is used to generate a Gaussian process regression model linking the inputs to the outputs. An advantage of the Gaussian process approach is the inherent quantification of uncertainty given by the model prediction.

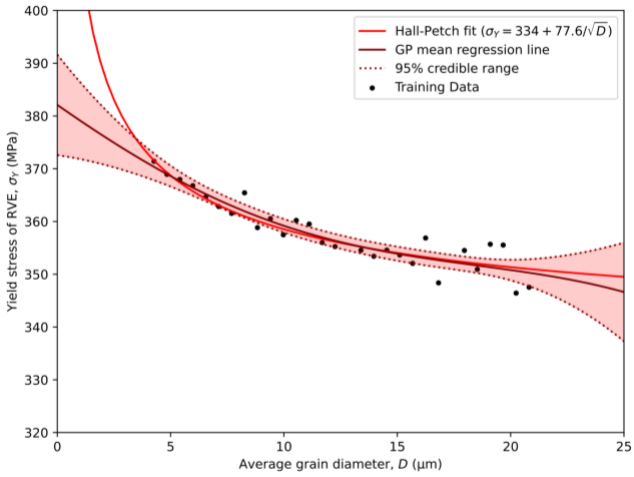
2. Results

The synthetic polycrystal representative volume elements (RVE) generated is shown in Figure 1a. The Experimental data and the calibrated crystal plasticity simulation is Figure 1b. Figure 1c shows the datapoints used to train the surrogate model and the mean Gaussian process regression line. More uncertainty in the prediction is observed outside the range within which the model was trained demonstrating that the while the model interpolates well, it is less precise in making predictions via extrapolation.

(a)



(b)



(c)

3. Conclusions

The Gaussian regression model extracted from CPFE results is an easy to use and fast model predicting the yield stress of the material as a function of its grainsize. It corresponds with a Hall-Petch phenomenological model validating its average result while providing uncertainty bands for the area it has been calibrated for but critically, for extrapolating where there is no data available. It demonstrates how surrogate models can be used to link microstructural parameters with macroscopic behaviour and how predictions can be made up and down these length scales providing a path for in-silico qualification of materials without need for costly large scale continuum size experimental programmes.

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