Efficient texture prediction using Gaussian process surrogate models

Michael Atkinson*[1], Pratheek Shanthraj[2], Tim Dodwell[3,4], and João Quinta Da Fonseca[1]

[1]Department of Materials, University of Manchester, UK – United Kingdom
[2]United Kingdom Atomic Energy Authority, UK – United Kingdom
[3]College of Engineering Mathematics and Physical Sciences, University of Exeter, UK – United Kingdom
[4]digilab, UK – United Kingdom

Abstract

Effective models of crystallographic texture development during thermomechanical processing can help speed up the introduction of new alloys, optimise current processing routes and catalyse new process development. Full-field crystal plasticity (CP) models with complex non-local constitutive laws are capable of accounting for variation of microstructure and its development. However, they are computationally expensive and cannot be run inline within forming process models or used to probe uncertainty arising from varied input parameters. Their computational expense also prohibits making predictions of the spatial distribution of texture in large components, by coupling a CP model with a process model for example. In this work, we have used Gaussian process (GP) regression to make efficient texture predictions during a forging process. Linking of CP to process models requires many calls to the CP model, often with very similar inputs. A GP can be used to create surrogate models within a known area of parameter space and encode the texture development information produced by the physical (CP) model at reduced order. Inputs and outputs of the model include texture represented as an ODF, loading condition and temperature. Careful consideration was taken to minimise the dimension of the representation of these parameters to ensure the surrogate was efficient in both memory and compute time. We find that the GP model can produce textures consistent with the CP models within the uncertainty introduced by the finite sampling of the ODF into a representative volume element (RVE). This accuracy is investigated when varying the size of the training set to minimise the number of CP simulation runs required. The GP is orders of magnitude quicker than the complex CP models and will allow an effective coupling of physical and process models.

Keywords: Surrogate model, Gaussian process, Crystal plasticity

*Speaker