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# Multi-scale modelling of stress-induced martensitic phase transformations

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## Abstract

Martensitic phase transformations play a crucial role in the mechanical behaviour of industrially important materials, such as austenitic stainless steels and TRIP (Transformation Induced Plasticity) steels. From a modelling perspective, they pose significant challenges because of a complex interplay, at the crystal lattice scale, between physical mechanisms involving volumetric expansion across multiple slip systems during the transformations. As such, the classical phenomenological approach to material modelling often falls short of appropriately predicting the deformation process of such materials. In this context, multi-scale models can help to elucidate the relationship between microscopic properties and the corresponding macroscopic material behaviour.

This work concerns the continued development and validation of a micromechanically-based constitutive model for materials undergoing stress-induced martensitic phase transformations, locally formulated to describe the crystal lattice transformations [1]. The model is cast from a physical metallurgical mechanism and derived from the principles of thermodynamics, inheriting a consistent mechanical dissipation. The transformation function is developed in multi-axial stress states that could be considered as a generalisation to the stress-assisted criterion introduced by Patel and Cohen (1953) for the uniaxial case. This plasticity-like elasto-viscoplastic microscopic model incorporates austenite viscoplasticity coupled with the irreversible austenite-to-martensite transformation, sharing many features with conventional finite strain crystal plasticity models. This model is incorporated into an RVE (Representative Volume Element), where a computational homogenisation scheme based on a fully implicit finite element method is employed to obtain the micro-to-macro transitions. Preliminary results in two-dimensions show agreement with experimentally obtained transformation surfaces [1]. Since the physical description of the crystal slip systems is inherently three-dimensional, the proposed extension of the current framework to fully 3-D simulations should provide promising results.

The resulting computational scheme allows for macro-scale stress-strain relationships to be obtained from the RVE level. These results can be used to aid the design of alloy microstructures that have certain desired properties, or in practical coupled macro-scale (FE<sup>2</sup>) simulations.

F. Adziman, "Constitutive modelling and finite element simulation of martensitic transformation using a computational multi-scale framework", PhD Thesis, Swansea University (2014).

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