A Multi-Scale Modeling of Multiphase Advanced High Strength Steels Based on Crystal Plasticity and Evolutionary Yield Function

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Abstract. A multi-scale modeling of multiphase advanced high strength steels was developed based on crystal plasticity and evolutionary yield function. An analytical model to directly predict the mechanical behavior of each phase was developed from crystal plasticity model and EBSD data. Considering the grain size and orientation distribution, evolution of the yield surface could be directly predicted by the analytical prediction model. The yield surface prediction results were applied to the evolutionary yield function model. Macroscopic mechanical behavior of the multiphase material could be predicted by considering the volume fraction of each phase, which enables to optimize the desired material properties during the development of the multiphase material.

1. Introduction
To reduce the amount of time and cost required for material and product design, computational approaches have been adopted to predict and evaluate the mechanical performance of materials, such as formability and springback. In particular, for the precise prediction of the mechanical behavior, advanced constitutive models are required to account for the macroscopic behavior observed from various experiments. Further endeavors have been made to develop advanced material models and to regenerate the microstructures to represent the microstructural behavior.

In this work, a multi-scale modeling of multiphase advanced high strength steels was developed based on crystal plasticity [1] and evolutionary yield function. As an alternative to the finite element approaches along with the generation of the 3D representative volume elements (RVE), an analytical model to directly predict the mechanical behavior of each phase from EBSD data was developed based on crystal plasticity. In the developed analytical prediction model, the stress-strain behavior and the evolution of the r-value and yield surface with respect to the plastic deformation could be directly predicted by considering the grain size distribution and orientation distribution obtained from the EBSD data. Then, the generated initial yield surface and its evolution were applied to calibrate the phenomenological evolutionary yield function model. A generalized J2 based non-quadratic asymmetric/anisotropic function was applied for the yield function.

By developing the analytical model, the impact that the volume fraction and material properties of each phase have on the macroscopic behavior could be directly predicted without performing finite...
element simulations. This will in turn reduce the total time required to optimize the desired material properties of a multiphase steel.

2. Development of an analytical model to directly predict yield surface based on crystal plasticity and measured EBSD data

An analytical model to directly predict the mechanical behavior of each phase from EBSD data was developed based on crystal plasticity. As schematically shown in Figure 1, the initial yield surface for each grain is calculated by considering the crystal orientation within a multiphase steel. The macroscopic yield surface is then obtained by homogenizing the yield surfaces for representative grain orientations. Figure 2 shows the comparison of the combined yield surface for BCC crystals by increasing the number of grains. In the crystal plasticity simulations, the crystal orientation for each grain was randomly generated and 24 slip systems were considered for BCC crystals (12 {110}<111> and 12 {112}). As the number of grains considered in the crystal plasticity simulation increases, the yield surface shape converges to the smooth isotropic yield surface.

Figure 3 shows the combined yield surface and its evolution generated by the developed analytical model utilizing the crystal orientations measured from EBSD data. For demonstration purposes, 1000 grains of BCC crystals were randomly selected from the EBSD data. For the generation of the initial yield surface, the number of crystal orientations within each grain was assumed, and then the yield surface evolution was calculated for different loading conditions. The work hardening rate for each slip system was obtained from the micro-pillar compression data.

Besides the calculation of the initial yield surface and its evolution, the macroscopic stress-strain behaviour, as well as the r-value evolution during the uniaxial tension were also predicted by the developed analytical model. Figure 4 shows the r-value evolutions during the uniaxial tension.

To evaluate the accuracy of the developed analytical model in predicting the global stress-strain curves, the crystal plasticity FE simulation was also performed to generate a uniaxial tension stress-strain curve. A hypothetical ferrite with 48 slip systems (12 {110}<111>, 12 {112} and 24 {123}<111> slip systems) was considered and the same hardening parameters were used both for the analytical crystal plasticity simulation and the CPFE simulation. A rectangular specimen shown in Figure 5 with randomly distributed BCC crystals were considered for the CPFE simulation. As shown in Figure 6, the
stress-strain curve generated by the developed analytical model is almost identical to the curves obtained by the CPFE simulation.

**Figure 3.** Calculated stress-strain curves during the uniaxial tension for different loading directions (BCC crystal).

**Figure 4.** Calculated r-value evolutions during the uniaxial tension for different loading directions (BCC crystal).

**Figure 5.** A rectangular specimen with randomly distributed BCC crystals used for the CPFE simulation.

**Figure 6.** Comparison of the obtained stress-strain curves from the CPFE simulation and the analytical model.

3. Implementation of predicted data into the evolutionary yield function model
The calculated yield surfaces for individual phases were utilized to generate the macroscopic yield surface and its evolution for a multiphase steel. In addition to crystal orientations, the volume fraction of each phase and grain size distributions, the grain shape distributions were also utilized in the generation of the macroscopic yield surface and its evolution. The results were then implemented into the phenomenological evolutionary yield function model [2].

As a demonstration, Figures 7 and 8 show the yield surface evolution and stress-strain curves for BAO QP980 steel represented by the phenomenological evolutionary yield function model. The evolution of the yield stress for each direction were characterized for the yield function using Yld2000-2D function. The calculated yield stresses during the uniaxial tension for different tensile directions are
compared with the measured yield stresses and showed reasonably good agreement, as shown in Figure 8.

**Figure 7.** Contours of the yield function for BAO QP980 steel

**Figure 8.** Comparison of the measured and simulated true stress-strain curves for the rolling, 45 and 90 degrees off tensile directions.

**Figure 9.** Comparison of the measured and simulated ultimate tensile strength distributions.

**References**

[1] Zamiri A and Pourboghrat F, 2010, *Int. J. Plast.* **26** 731-46

[2] Zamiri A and Pourboghrat F, 2007, *Int. J. Solid Struc.* **44** 8627-47